Non-Equilibrium Continuum Physics

Extended lecture notes by Eran Bouchbinder

(Dated: July 10, 2023)

This course is intended to introduce graduate students to the essentials of modern continuum physics, with a focus on non-equilibrium phenomena in solids and within a thermodynamic perspective. Special focus is given to emergent phenomena, where collective many-body systems reveal physical principles that cannot be inferred from the microscopic physics of a small number of degrees of freedom. General concepts and principles — such as conservation laws, symmetries, material frame-indifference, dissipation inequalities and non-equilibrium behaviors, spatiotemporal symmetry-breaking instabilities and configurational forces — are emphasized. Examples cover a wide range of physical phenomena and applications in diverse disciplines. The power of field theory as a mathematical structure that does not make direct reference to microscopic length scales well below those of the phenomenon of interest is highlighted. Some basic mathematical tools and techniques are introduced. The course highlights essential ideas and basic physical intuition. Together with courses on fluid mechanics and soft condensed matter, a broad background and understanding of continuum physics will be established.

The course will be given within a framework of 12-13 two-hour lectures and 12-13 two-hour tutorial sessions with a focus on problem-solving. No prior knowledge of the subject is assumed. Basic knowledge of statistical thermodynamics, vector calculus, partial differential equations, dynamical systems and complex analysis is required.

These extended lecture notes (book draft) are self-contained and in principle no other materials are needed.

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Lectures: Tuesday, 11:15–13:00, Weissman, Seminar Rm A

Tutorials: Wednesday, 11:15–13:00, Weissman, Seminar Rm A

Final grade:

About 7 problems sets throughout the semester (40%) and final exam/assignment (60%).

Attendance:

Expected and highly encouraged (both lectures and tutorial sessions).

General Principles and Concepts

I.   INTRODUCTION: BACKGROUND AND MOTIVATION

We start by considering the course's title. By 'non-equilibrium' we refer to physical phenomena that cannot be properly treated in the framework of equilibrium thermodynamics. That is, we refer to phenomena that involve irreversible processes and dissipation. We will, however, make an effort to adhere as much as possible to thermodynamic formulations (i.e. we will not focus on purely dynamical systems) and also devote time to reversible phenomena (both because they are often missing from current physics education and because they set the stage for discussing irreversible phenomena). By 'continuum' we refer to the scientific approach that treats macroscopic phenomena without making explicit reference to the discreteness of matter or more generally to microscopic length and time scales. This also implies that we focus on collective phenomena that involve spatially extended systems and a macroscopic number of degrees of freedom (atoms, molecules, grains etc.). We therefore treat materials as continua and use the language of field theory to describe the phenomena of interest. A crucial concept in this context is that of emergent phenomena, which refers to the fundamental idea that collective many-body systems reveal laws/behavior that cannot be inferred from microscopic laws of physics and a small number of degrees of freedom; that is, "More is Different", adopting the famous title of Philip W. Anderson (see Science **177**, 393 (1972)).

'Physics' is surely a bit too broad here, yet it represents the idea that the tools and concepts that will be discussed have a very broad range of applications in different branches of physics. In addition, the topics considered can be discussed from various perspectives — such as applied mathematics, engineering sciences and materials science —, but we will adopt a physicist perspective. To make 'physics' even more specific in the present context, we note that we will mainly focus on thermal and mechanical phenomena, rather than electrical, magnetic or chemical phenomena. By 'thermal' and 'mechanical' — or 'thermomechanical' we refer to material phenomena that involve deformation, material and heat flow and failure, and where the driving forces are thermal and mechanical in nature. 'Classical continuum mechanics' typically refers to 'solid mechanics' and 'fluid mechanics' from a classical (i.e. non-quantum) physics perspective. In this course we will mainly focus on solids in the broadest sense of the word.

The word 'solid' is not easily defined. The most intricate aspect of such a definition is that it

involves an observation timescale (at least if we do not consider single crystals). However, for the purpose of this course, it will be sufficient to define a solid as a material that can support shear forces over sufficiently long timescales. We therefore do not focus on Newtonian fluids and very soft materials (though we certainly mention them), both of which are discussed in complementary courses. Nevertheless, we will discuss solid phenomena such as visco-elasticity and nonlinear elasticity.

Why should one study the subjects taught in this course? Well, there are many (good) reasons. Let us mention a few of them. First, macroscopic physics deals with emergent phenomena that cannot be understood from microscopic laws applied to a small number of constituent elements (degrees of freedom). That is, macroscopic systems feature new qualitative coarse-grained properties and dynamics. This is a deep conceptual, to some extent even philosophical, issue that should be systematically introduced. Second, many of the macroscopic phenomena around us are both non-equilibrium and thermomechanical in nature. This course offers tools to understand some of these phenomena. Third, continuum physics phenomena, and solid-related phenomena in particular, are ubiquitous in many branches of science and therefore understanding them may be very useful for researchers in a broad range of disciplines. Fourth, the conceptual and mathematical tools of non-equilibrium thermodynamics and field theory are extremely useful in many branches of science, and thus constitute an important part of scientific education. Finally, some of the issues discussed in this course are related to several outstanding unsolved problems. Hence, the course will expose students to the beauty and depth of a fundamental and active field of research. It would be impossible to even scratch the surface of the huge ongoing solid-related activity. Let us mention a few examples: **(i)** It has been quite recently recognized that the mechanics of living matter, cells in particular, plays a central role in biology. For example, it has been discovered that the stiffness of the substrate on which stem cells grow can significantly affect their differentiation. **(ii)** Biomimetics: researchers have realized that natural/biological systems exhibit superior mechanical properties, and hence aim at mimicking the design principles of these systems in man-made ones. For example, people have managed to build superior adhesives based on Gecko's motion on a wall. People have succeeded in synthesizing better composite materials based on the structures observed in hard tissues, such as cortical bone and dentin. **(iii)** The efforts to understand the physics of driven disordered systems (granular materials, molecular glasses, colloidal suspensions etc.) are deeply related to one of the most outstanding questions in non-equilibrium statistical physics. **(iv)** People have recently realized there are intimate relations

between geometry and mechanics. For example, by controlling the intrinsic metric of materials, macroscopic shapes can be explained and designed. **(v)** The rupture of materials and interfaces has a growing influence on our understanding and control of the world around us. For example, there are exciting developments in understanding Earthquakes, the failure of interfaces between two tectonic plates in the Earth's crust **(vi)** Developments in understanding the plastic deformation of amorphous and crystalline solids offer deep new insights about strongly nonlinear and dissipative systems, and open the way to new and exciting applications.

Unfortunately, due to time limitations, the course cannot follow a *historical perspective* which highlights the evolution of the developed ideas. These may provide very important scientific, sociological and psychological insights, especially for research students and young researchers. Whenever possible, historical notes will be made.

II. MATHEMATICAL PRELIMINARIES: TENSOR ANALYSIS

The fundamental assumption of continuum physics is that under a wide range of conditions we can treat materials as *continuous* in space and time, disregarding their discrete structure and time-evolution at microscopic length and time scales, respectively. Therefore, we can ascribe to each point in space-time physical properties that can be described by continuous functions, i.e. *fields*. This implies that derivatives are well defined and hence that we can use the powerful tools of differential calculus. In order to understand what kind of continuous functions, hereafter termed fields, should be used, we should bear in mind that physical laws must be independent of the position and orientation of an observer, and the time of observation (note that we restrict ourselves to classical physics, excluding the theory of relativity). We are concerned here, however, with the mathematical objects that allow us to formulate this and related principles. Most generally, we are interested in the language that naturally allows a mathematical formulation of continuum physical laws. The basic ingredients in this language are *tensor fields*, which are the major focus on the opening part of the course.

Tensor fields are characterized, among other things, by their *order* (sometimes also termed *rank*). Zero-order tensors are *scalars*, for example the temperature field $T(\boldsymbol{x}, t)$ within a body, where $\boldsymbol{x}$ is a 3-dimensional Euclidean space and t is time. First-order tensors are *vectors*, for example the velocity field $\boldsymbol{v}(\boldsymbol{x}, t)$ of a fluid. **Why do we need to consider objects that are higher-order than vectors?** The best way to answer this question is through an example. Consider a material areal element and the force acting on it (if the material areal element is a surface element, then the force is applied externally and if the material areal element is inside the bulk material, then the force is exerted by neighboring material). The point is that both the areal element and the force acting on it are basically vectors, i.e. they both have an orientation (the orientation of the areal element is usually quantified by the direction of the normal to it). Therefore, in order to characterize this physical situation one should say that a force in the ith direction is acting on a material areal element whose normal points in the jth direction. The resulting object is defined using two vectors, but it is not a vector itself. We need a higher-order tensor to describe it.

Our main interest here is second-order tensors, which play a major role in continuum physics. A second-order tensor $\boldsymbol{A}$ can be viewed as a linear operator or a linear function that maps a vector, say $\boldsymbol{u}$, to a vector, say $\boldsymbol{v}$,

$$\boldsymbol{v} = \boldsymbol{A}\boldsymbol{u} \ . \tag{2.1}$$

Linearity implies that

$$\boldsymbol{A}(\alpha\boldsymbol{u}+\boldsymbol{v})=\alpha\boldsymbol{A}\boldsymbol{u}+\boldsymbol{A}\boldsymbol{v}\;, \tag{2.2}$$

for every scalar α and vectors $\boldsymbol{u}$ and $\boldsymbol{v}$. For brevity, second-order tensors will be usually referred to simply as tensors (zero-order tensors will be termed scalars, first-order tensors will be termed vectors and higher than second-order tensors will be explicitly referred to according to their order).

The most natural way to define (or express) tensors in terms of vectors is through the *dyadic* (or *tensor*) product of orthonormal base vectors $\{\boldsymbol{e}_i\}$

$$\boldsymbol{A}=A_{ij}\,\boldsymbol{e}_i\otimes\boldsymbol{e}_j\;, \tag{2.3}$$

where Einstein summation convention is adopted, $\{A_{ij}\}$ is a set of numbers and $\{i,j\}$ run over space dimensions. For those who feel more comfortable with Dirac's Bra-Ket notation, the dyadic product above can be also written as $\boldsymbol{A}=A_{ij}\,|e_i><e_j|$. In general, the dyad $\boldsymbol{u}\otimes\boldsymbol{v}$ is defined as

$$\boldsymbol{u}\otimes\boldsymbol{v}=\boldsymbol{u}\boldsymbol{v}^T\;, \tag{2.4}$$

where vectors are assumed to be represented by column vectors and the superscript T denotes the transpose operation. If $\{\boldsymbol{e}_i\}$ is an orthonormal set of Cartesian base vectors, we have (for example)

$$\boldsymbol{e}_2\otimes\boldsymbol{e}_3=\boldsymbol{e}_2\boldsymbol{e}_3^T=\begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0&0&1\end{pmatrix}=\begin{pmatrix}0&0&0\\0&0&1\\0&0&0\end{pmatrix}\;. \tag{2.5}$$

Therefore, second-order tensors can be directly *represented* by matrices. Thus, tensor algebra essentially reduces to matrix algebra. It is useful to note that for every three vectors $\boldsymbol{u}$, $\boldsymbol{v}$ and $\boldsymbol{w}$ we have

$$\boldsymbol{u}\otimes\boldsymbol{v}\,\boldsymbol{w}=(\boldsymbol{v}\cdot\boldsymbol{w})\,\boldsymbol{u}\;. \tag{2.6}$$

where $\cdot$ is the usual inner (dot) product of vectors. In the Bra-Ket notation the above simply reads $|\boldsymbol{u}><\boldsymbol{v}|\boldsymbol{w}>$ This immediately allows us to rewrite Eq. (2.1) as

$$v_i\boldsymbol{e}_i=\boldsymbol{v}=\boldsymbol{A}\boldsymbol{u}=(A_{ij}\boldsymbol{e}_i\otimes\boldsymbol{e}_j)(u_k\boldsymbol{e}_k)=A_{ij}u_k(\boldsymbol{e}_j\cdot\boldsymbol{e}_k)\,\boldsymbol{e}_i=A_{ij}u_j\boldsymbol{e}_i\;, \tag{2.7}$$

which shows that the matrix representation preserves known properties of matrix algebra ($v_i=A_{ij}u_j$). The matrix representation allows us to define additional tensorial operators. For example,

we can define

$$\text{tr}(\boldsymbol{A}) \equiv \boldsymbol{e}_k \cdot (A_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j)\,\boldsymbol{e}_k = A_{ij} <\boldsymbol{e}_k|\boldsymbol{e}_i><\boldsymbol{e}_j|\boldsymbol{e}_k> = A_{ij}\delta_{ik}\delta_{jk} = A_{kk} \ , \tag{2.8}$$

$$\boldsymbol{A}^T = (A_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j)^T = A_{ij}\boldsymbol{e}_j \otimes \boldsymbol{e}_i = A_{ji}\boldsymbol{e}_i \otimes \boldsymbol{e}_j \ , \tag{2.9}$$

$$\boldsymbol{AB} = (A_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j)(B_{kl}\boldsymbol{e}_k \otimes \boldsymbol{e}_l) = A_{ij}B_{kl}\delta_{jk}\boldsymbol{e}_i \otimes \boldsymbol{e}_l = A_{ij}B_{jl}\boldsymbol{e}_i \otimes \boldsymbol{e}_l \ . \tag{2.10}$$

We can define the *double dot product* (or the *contraction*) of two tensors as

$$\boldsymbol{A} : \boldsymbol{B} = (A_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j) : (B_{kl}\boldsymbol{e}_k \otimes \boldsymbol{e}_l) \equiv A_{ij}B_{kl}(\boldsymbol{e}_i \cdot \boldsymbol{e}_k)(\boldsymbol{e}_j \cdot \boldsymbol{e}_l)$$

$$= A_{ij}B_{kl}\delta_{ik}\delta_{jl} = A_{ij}B_{ij} = \text{tr}(\boldsymbol{A}\,\boldsymbol{B}^T) \ . \tag{2.11}$$

This is a natural way of generating a scalar out of two tensors, which is the tensorial generalization of the usual vectorial dot product (hence the name). It plays an important role in the thermodynamics of deforming bodies. Furthermore, it allows us to project a tensor on a base dyad

$$(\boldsymbol{e}_i \otimes \boldsymbol{e}_j) : \boldsymbol{A} = (\boldsymbol{e}_i \otimes \boldsymbol{e}_j) : (A_{kl}\boldsymbol{e}_k \otimes \boldsymbol{e}_l) = A_{kl}(\boldsymbol{e}_i \cdot \boldsymbol{e}_k)(\boldsymbol{e}_j \cdot \boldsymbol{e}_l) = A_{kl}\delta_{ik}\delta_{jl} = A_{ij} \ , \tag{2.12}$$

i.e. to extract a component of a tensor.

We can now define the identity tensor as

$$\boldsymbol{I} = \delta_{ij}(\boldsymbol{e}_i \otimes \boldsymbol{e}_j) \ , \tag{2.13}$$

which immediately allows to define the inverse of a tensor (when it exists) following

$$\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{I} \ . \tag{2.14}$$

The existence of the inverse is guaranteed when $\det \boldsymbol{A} \neq 0$, where the determinant of a tensor is defined using the determinant of its matrix representation. Note also that one can decompose any second-order tensor to a sum of symmetric and skew-symmetric (antisymmetric) parts as

$$\boldsymbol{A} = \boldsymbol{A}_{sym} + \boldsymbol{A}_{skew} = \frac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^T) + \frac{1}{2}(\boldsymbol{A} - \boldsymbol{A}^T) \ . \tag{2.15}$$

Occasionally, physical constraints render the tensors of interest symmetric, i.e. $\boldsymbol{A} = \boldsymbol{A}^T$. In this case, we can diagonalize the tensor by formulating the eigenvalue problem

$$\boldsymbol{A}\boldsymbol{a}_i = \lambda_i \boldsymbol{a}_i \ , \tag{2.16}$$

where $\{\lambda_i\}$ and $\{\boldsymbol{a}_i\}$ are the eigenvalues (principal values) and the orthonormal eigenvectors (principal directions), respectively. This problem is analogous to finding the roots of

$$\det(\boldsymbol{A} - \lambda\boldsymbol{I}) = -\lambda^3 + \lambda^2 I_1(\boldsymbol{A}) - \lambda I_2(\boldsymbol{A}) + I_3(\boldsymbol{A}) = 0 \ , \tag{2.17}$$

where the *principal invariants* $\{I_i(\boldsymbol{A})\}$ are given by

$$I_1(\boldsymbol{A}) = \mathrm{tr}(\boldsymbol{A}), \quad I_2(\boldsymbol{A}) = \frac{1}{2}\left[\mathrm{tr}^2(\boldsymbol{A}) - \mathrm{tr}(\boldsymbol{A}^2)\right], \quad I_3(\boldsymbol{A}) = \det(\boldsymbol{A}) . \tag{2.18}$$

Note that the symmetry of $\boldsymbol{A}$ ensures that the eigenvalues are real and that an orthonormal set of eigenvectors can be constructed. Therefore, we can represent any symmetric tensor as

$$\boldsymbol{A} = \lambda_i \, \boldsymbol{a}_i \otimes \boldsymbol{a}_i , \tag{2.19}$$

assuming no degeneracy. This is called the *spectral decomposition* of a symmetric tensor $\boldsymbol{A}$. It is very useful because it represents a tensor by 3 real numbers and 3 unit vectors. It also allows us to define functions of tensors. For example, for positive definite tensors ($\lambda_i > 0$), we can define

$$\ln(\boldsymbol{A}) = \ln(\lambda_i) \, \boldsymbol{a}_i \otimes \boldsymbol{a}_i , \tag{2.20}$$

$$\sqrt{\boldsymbol{A}} = \sqrt{\lambda_i} \, \boldsymbol{a}_i \otimes \boldsymbol{a}_i . \tag{2.21}$$

In general, one can define functions of tensors that are themselves scalars, vectors or tensors. Consider, for example, a scalar function of a tensor $f(\boldsymbol{A})$ (e.g. the energy density of a deforming solid). Consequently, we need to consider *tensor calculus*. For example, the derivative of $f(\boldsymbol{A})$ with respect to $\boldsymbol{A}$ is a tensor which takes the form

$$\frac{\partial f}{\partial \boldsymbol{A}} = \frac{\partial f}{\partial A_{ij}} \boldsymbol{e}_i \otimes \boldsymbol{e}_j . \tag{2.22}$$

The differential of $f(\boldsymbol{A})$ is a scalar and reads

$$df = \frac{\partial f}{\partial \boldsymbol{A}} : d\boldsymbol{A} = \frac{\partial f}{\partial A_{ij}} dA_{ij} . \tag{2.23}$$

Consider then a tensorial function of a tensor $\boldsymbol{F}(\boldsymbol{A})$, which is encountered quite regularly in continuum physics. Its derivative $\boldsymbol{D}$ is defined as

$$\boldsymbol{D} = \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{A}} = \frac{\partial \boldsymbol{F}}{\partial A_{ij}} \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j = \frac{\partial F_{kl}}{\partial A_{ij}} \boldsymbol{e}_k \otimes \boldsymbol{e}_l \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j ,$$

$$\implies D_{klij} = \frac{\partial F_{kl}}{\partial A_{ij}} , \tag{2.24}$$

which is a fourth-order tensor.

We will now define some differential operators that either produce tensors or act on tensors. First, consider a vector field $\boldsymbol{v}(\boldsymbol{x})$ and define its gradient as

$$\nabla \boldsymbol{v} = \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{v}}{\partial x_j} \otimes \boldsymbol{e}_j = \frac{\partial v_i}{\partial x_j} \boldsymbol{e}_i \otimes \boldsymbol{e}_j , \tag{2.25}$$

which is a second-order tensor. Then, consider the divergence of a tensor

$$\nabla \cdot \boldsymbol{A} = \frac{\partial \boldsymbol{A}}{\partial x_k} \boldsymbol{e}_k = \frac{\partial A_{ij}}{\partial x_k} \boldsymbol{e}_i \otimes \boldsymbol{e}_j \boldsymbol{e}_k = \frac{\partial A_{ij}}{\partial x_j} \boldsymbol{e}_i \ , \tag{2.26}$$

which is a vector. The last two objects are extensively used in continuum physics.

The tensorial version of Gauss' theorem for relating volume integrals to surface integrals reads

$$\int_V \nabla \cdot \boldsymbol{A} \, dV = \oint_S \boldsymbol{A} \boldsymbol{n} \, dS \ , \tag{2.27}$$

where V and S are the volume and the enclosing surface, respectively, and $\boldsymbol{n}$ is the outward unit normal to the surface. Obviously, the theorem is satisfied for scalars and vectors as well. It would be useful to recall also Stokes' theorem for relating line integrals to surface integrals

$$\int_S (\nabla \times \boldsymbol{v}) \cdot \boldsymbol{n} dS = \oint_l \boldsymbol{v} \cdot d\boldsymbol{l} \ , \tag{2.28}$$

where S and l are the surface and its bounding curve, respectively, and $\boldsymbol{n}$ is the outward unit normal to the surface.

Finally, we should ask ourselves how do tensors transform under a coordinate transformation (from $\boldsymbol{x}$ to $\boldsymbol{x}'$)

$$\boldsymbol{x}' = \boldsymbol{Q} \boldsymbol{x} \ , \tag{2.29}$$

where $\boldsymbol{Q}$ is a proper ($\det \boldsymbol{Q} = 1$) orthogonal transformation matrix $\boldsymbol{Q}^T = \boldsymbol{Q}^{-1}$ (note that it is not a tensor). In order to understand the transformation properties of the orthonormal base vectors $\{\boldsymbol{e}_i\}$ we first note that

$$\boldsymbol{x}' = \boldsymbol{Q} \boldsymbol{x} \implies \boldsymbol{x} = \boldsymbol{Q}^T \boldsymbol{x}' \implies x_i = Q^T_{ij} x'_j = Q_{ji} x'_j \ . \tag{2.30}$$

A vector is an object that retains its (geometric) identity under a coordinate transformation. For example, a general position vector $\boldsymbol{r}$ can be *represented* using two different base vectors sets $\{\boldsymbol{e}_i\}$ and $\{\boldsymbol{e}'_i\}$ as

$$\boldsymbol{r} = x_i \boldsymbol{e}_i = x'_j \boldsymbol{e}'_j \ . \tag{2.31}$$

Using Eq. (2.30) we obtain

$$x_i \boldsymbol{e}_i = (Q_{ji} x'_j) \boldsymbol{e}_i = x'_j (Q_{ji} \boldsymbol{e}_i) = x'_j \boldsymbol{e}'_j \ , \tag{2.32}$$

which implies

$$\boldsymbol{e}'_i = Q_{ij} \boldsymbol{e}_j \ . \tag{2.33}$$

In order to derive the transformation law for tensors representation we first note that tensors, like vectors, are objects that retain their (geometric) identity under a coordinate transformation and therefore we must have

$$\boldsymbol{A} = A_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j = A'_{ij}\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j \ . \tag{2.34}$$

Using Eq. (2.33) we obtain

$$\boldsymbol{A} = A'_{ij}\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j = A'_{ij}Q_{ik}\boldsymbol{e}_k \otimes Q_{jl}\boldsymbol{e}_l = (A'_{ij}Q_{ik}Q_{jl})\boldsymbol{e}_k \otimes \boldsymbol{e}_l \ . \tag{2.35}$$

which implies

$$A_{kl} = A'_{ij}Q_{ik}Q_{jl} \ . \tag{2.36}$$

This is the transformation law for the components of a tensor and in many textbooks it serves as a definition of a tensor. Eq. (2.36) can be written in terms of matrix representation as

$$[\boldsymbol{A}] = \boldsymbol{Q}^T[\boldsymbol{A}]'\boldsymbol{Q} \Longrightarrow [\boldsymbol{A}]' = \boldsymbol{Q}[\boldsymbol{A}]\boldsymbol{Q}^T \ , \tag{2.37}$$

where $[\cdot]$ is the matrix representation of a tensor with respect to a set of base vectors. Though we did not make the explicit distinction between a tensor and its matrix representation earlier, it is important in the present context; $[\boldsymbol{A}]$ and $[\boldsymbol{A}]'$ are different representations of the same object, the tensor $\boldsymbol{A}$, but **not** different tensors. An isotropic tensor is a tensor whose representation is independent of the coordinate system, i.e.

$$A_{ij} = A'_{ij} \quad \text{or} \quad [\boldsymbol{A}] = [\boldsymbol{A}]' \ . \tag{2.38}$$

We note in passing that in the present context we do not distinguish between covariant and contravariant tensors, a distinction that is relevant for non-Cartesian tensors (a *Cartesian tensor* is a tensor in three-dimensional Euclidean space for which a coordinate transformation $\boldsymbol{x}' = \boldsymbol{Q}\boldsymbol{x}$ satisfies $\partial x'_i/\partial x_j = \partial x_j/\partial x'_i$).

III. MOTION, DEFORMATION AND STRESS

Solid materials are deformed under applied driving forces. In order to describe the deformation of solids, consider a body at a given time and assign to each material point a position vector $\boldsymbol{X}$ with respect to some fixed coordinate system (i.e. we already use the continuum assumption). For simplicity, set $t=0$. At $t>0$ the body experiences some external forcing that deforms it to a state in which each material point is described by a position vector $\boldsymbol{x}$. We then define the **motion** as the following mapping

$$\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{X},t) = \boldsymbol{\varphi}(\boldsymbol{X},t) \ . \tag{3.1}$$

The vector function $\boldsymbol{\varphi}(\cdot)$ maps each point in the initial state $\boldsymbol{X}$ to a point in the current state $\boldsymbol{x}$ at $t>0$. This immediately implies that $\boldsymbol{X} = \boldsymbol{\varphi}(\boldsymbol{X}, t = 0)$, i.e. at time $t = 0$ $\boldsymbol{\varphi}(\cdot)$ is the identity vector. The initial state $\boldsymbol{X}$ is usually termed the *reference/undeformed configuration* and the current state is termed the *deformed configuration*. We assume that $\boldsymbol{\varphi}(\cdot)$ is a one-to-one mapping, i.e. that it can be inverted

$$\boldsymbol{X} = \boldsymbol{\varphi}^{-1}(\boldsymbol{x},t) \ . \tag{3.2}$$

The inverse mapping $\boldsymbol{\varphi}^{-1}(\cdot)$ tells us where a material point, that is currently at $\boldsymbol{x}$, was at time $t = 0$. It is important to note that we can describe physical quantities either by $\boldsymbol{X}$, which is called the *material (Lagrangian) description*, or by $\boldsymbol{x}$, which is called the *spatial (Eulerian) description*. The choice between these descriptions is a matter of convenience. For a given physical phenomenon under consideration, one description may be more convenient than the other. We will discuss this issue later in the course.

A quantity of fundamental importance is the *displacement field* defined as

$$\boldsymbol{U}(\boldsymbol{X},t) = \boldsymbol{x}(\boldsymbol{X},t) - \boldsymbol{X} \ . \tag{3.3}$$

This material description can be converted into a spatial description following

$$\boldsymbol{U}(\boldsymbol{X},t) = \boldsymbol{x}(\boldsymbol{X},t) - \boldsymbol{X} = \boldsymbol{x} - \boldsymbol{X}(\boldsymbol{x},t) = \boldsymbol{U}(\boldsymbol{\varphi}^{-1}(\boldsymbol{x},t),t) = \boldsymbol{u}(\boldsymbol{x},t) \ . \tag{3.4}$$

Note that $\boldsymbol{U}$ and $\boldsymbol{u}$ are different functions of different arguments, though their values are the same. The velocity and acceleration fields are defined as

$$\boldsymbol{V}(\boldsymbol{X},t) = \partial_t \boldsymbol{U}(\boldsymbol{X},t) = \boldsymbol{v}(\boldsymbol{x},t) \quad \text{and} \quad \boldsymbol{A}(\boldsymbol{X},t) = \partial_{tt} \boldsymbol{U}(\boldsymbol{X},t) = \boldsymbol{a}(\boldsymbol{x},t) \ . \tag{3.5}$$

The corresponding spatial descriptions can be easily obtained using $\boldsymbol{\varphi}(\cdot)$.

The material time derivative D/Dt, which we abbreviate by D_t, is defined as the partial derivative with respect to time, keeping the Lagrangian coordinate $\boldsymbol{X}$ fixed. For a material field $\mathcal{F}(\boldsymbol{X}, t)$ (scalar or vector. For a tensor, see the discussion of objectivity/frame-indifference later in the course) we have

$$D_t \mathcal{F}(\boldsymbol{X}, t) \equiv (\partial_t \mathcal{F}(\boldsymbol{X}, t))_{\boldsymbol{X}} \; , \tag{3.6}$$

where we stress that $\boldsymbol{X}$ is held fixed here. This derivative represents the time rate of change of a field $\mathcal{F}$, as seen by an observer moving with a particle that was at $\boldsymbol{X}$ at time $t = 0$. We can then ask ourselves what happens when we operate with the material derivative on an Eulerian field $f(\boldsymbol{x}, t)$. Using the definition in Eq. (3.6), we obtain

$$\begin{aligned}
\frac{Df(\boldsymbol{x}, t)}{Dt} &= \left(\frac{\partial f(\boldsymbol{\varphi}(\boldsymbol{X}, t), t)}{\partial t} \right)_{\boldsymbol{X} = \boldsymbol{\varphi}^{-1}(\boldsymbol{x}, t)} \\
&= \left(\frac{\partial f(\boldsymbol{x}, t)}{\partial t} \right)_{\boldsymbol{x}} + \left(\frac{\partial f(\boldsymbol{x}, t)}{\partial \boldsymbol{x}} \right)_t \left(\frac{\partial \boldsymbol{\varphi}(\boldsymbol{X}, t)}{\partial t} \right)_{\boldsymbol{X} = \boldsymbol{\varphi}^{-1}(\boldsymbol{x}, t)} \; .
\end{aligned} \tag{3.7}$$

The last term in the above expression is the velocity field, cf. Eq. (3.5), implying that

$$\frac{D(\cdots)}{Dt} = \frac{\partial(\cdots)}{\partial t} + v_k \frac{\partial(\cdots)}{\partial x_k} \; . \tag{3.8}$$

The second contribution on the right hand side of the above equation is termed the *convective rate of change* and hence the material derivative of an Eulerian field is sometimes called the *convective derivative*. Finally, note that since the material derivative of an Eulerian field is just the total time derivative of the Eulerian field, viewing $\boldsymbol{x}(t)$ as a function of time, it is sometimes denoted by a superimposed dot, i.e. $\dot{f}(\boldsymbol{x}, t) = D_t f(\boldsymbol{x}, t)$. If $f(\boldsymbol{x}, t)$ is the velocity field we obtain

$$D_t \boldsymbol{v}(\boldsymbol{x}, t) = \partial_t \boldsymbol{v}(\boldsymbol{x}, t) + \boldsymbol{v}(\boldsymbol{x}, t) \cdot \nabla_{\boldsymbol{x}} \boldsymbol{v}(\boldsymbol{x}, t) \; . \tag{3.9}$$

The latter nonlinearity is very important in fluid mechanics, though it appears also in the context of elasto-plasticity. Note that we distinguish between the *spatial gradient* $\nabla_{\boldsymbol{x}}$ and the *material gradient* $\nabla_{\boldsymbol{X}}$, which are different differential operators. Fluid flows are usually described using an Eulerian description. Nevertheless, Lagrangian formulations can be revealing, see for example the Lagrangian turbulence simulation at: http://www.youtube.com/watch?v=LHIIn72dRPk

In order to discuss the physics of deformation we need to know how material line elements change their length and orientation. Therefore, we define the *deformation gradient* $\boldsymbol{F}$ that maps an infinitesimal line element in the reference configuration $d\boldsymbol{X}$ to an infinitesimal line element in the deformed configuration

$$d\boldsymbol{x} = \boldsymbol{F}(\boldsymbol{X}, t) d\boldsymbol{X} \; . \tag{3.10}$$

Hence,

$$\boldsymbol{F}(\boldsymbol{X},t) = \nabla_{\boldsymbol{X}}\boldsymbol{\varphi}(\boldsymbol{X},t) \ . \tag{3.11}$$

As will become apparent later in the course, $\boldsymbol{F}$ is not a proper tensor, but rather a two-point tensor, i.e. a tensor that relates two configurations. We can further define the *displacement gradient tensor* as

$$\boldsymbol{H}(\boldsymbol{X},t) = \nabla_{\boldsymbol{X}}\boldsymbol{U}(\boldsymbol{X},t) \ , \tag{3.12}$$

which implies

$$\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{H} \ . \tag{3.13}$$

Here and elsewhere $\boldsymbol{I}$ is the identity tensor. The deformation gradient $\boldsymbol{F}$ describes both the rotation and the stretching of a material line element, which also implies that it is not symmetric. From a basic physics perspective, it is clear that interaction potentials are sensitive to the relative distance between particles, but not to local rigid rotations. Consequently, we are interested in separating rotations from stretching, where the latter quantifies the change in length of material elements. We can, therefore, decompose $\boldsymbol{F}$ as

$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U} = \boldsymbol{V}\boldsymbol{R} \ , \tag{3.14}$$

where $\boldsymbol{R}$ is a proper rotation tensor, $\det \boldsymbol{R} = +1$, and $\boldsymbol{U}$ (should not be confused with the displacement field) and $\boldsymbol{V}$ are the right and left stretch tensors, respectively (which are of course symmetric). This is the so-called *polar decomposition*. Note that

$$\boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{I}, \quad \boldsymbol{U} = \boldsymbol{U}^T, \quad \boldsymbol{V} = \boldsymbol{V}^T, \quad \boldsymbol{V} = \boldsymbol{R}\boldsymbol{U}\boldsymbol{R}^T \ . \tag{3.15}$$

Therefore, $\boldsymbol{U}$ and $\boldsymbol{V}$ have the same eigenvalues (principal stretches), but different eigenvectors (principal directions). Hence, we can write the spectral decomposition as

$$\boldsymbol{V} = \lambda_i \, \boldsymbol{N}_i \otimes \boldsymbol{N}_i, \tag{3.16}$$

$$\boldsymbol{U} = \lambda_i \, \boldsymbol{M}_i \otimes \boldsymbol{M}_i, \tag{3.17}$$

with

$$\lambda_i > 0, \quad \boldsymbol{N}_i \otimes \boldsymbol{N}_i = \boldsymbol{R}\boldsymbol{M}_i \otimes \boldsymbol{R}\boldsymbol{M}_i \ . \tag{3.18}$$

A. Strain measures

At this stage, we are interested in constructing quantities that are based on the stretch tensors discussed above in order to be able, eventually, to define the energy of deformation. For this aim, we need to discuss strain measures. Unlike displacements and stretches, which are directly measurable quantities (whether it always make physical sense and over which timescales, will be discussed later), *strain measures* are *concepts* that are defined based on displacements/stretches, and may be conveniently chosen differently in different physical situations. The basic idea is simple; we would like to come up with a measure of the relative change in length of material line elements. Consider first the scalar (one-dimensional) case. If the reference length of a material element is ℓ_0 and its deformed length is $\ell = \lambda \ell_0$, then a simple strain measure is constructed by

$$g(\lambda) = \frac{\ell - \ell_0}{\ell_0} = \lambda - 1 \ . \tag{3.19}$$

This definition follows our intuitive notion of strain, i.e. (i) It is a monotonically increasing function of the stretch λ (ii) It vanishes when $\lambda = 1$. It is, however, by no means unique. In fact, every monotonically increasing function of λ which reduces to the above definition when λ is close to unity, i.e. satisfies $g(1) = 0$ and $g'(1) = 1$, would qualify. These conditions ensure that upon linearization, all strain measures agree. For example,

$$g(\lambda) = \int_{\ell_0}^{\ell} \frac{d\ell'}{\ell'} = \ln\left(\frac{\ell}{\ell_0}\right) = \ln \lambda \ , \tag{3.20}$$

$$g(\lambda) = \frac{\ell^2 - \ell_0^2}{2\ell_0^2} = \frac{1}{2}\left(\lambda^2 - 1\right) \ . \tag{3.21}$$

Obviously, there are infinitely many more. The three possibilities we presented above, however, are well-motivated from a physical point of view. Before explaining this, we note that the scalar (one-dimensional) definitions adopted above can be easily generalized to rotationally invariant tensorial forms as

$$\boldsymbol{E}_B = (\lambda_i - 1)\, \boldsymbol{M}_i \otimes \boldsymbol{M}_i = \boldsymbol{U} - \boldsymbol{I}, \tag{3.22}$$

$$\boldsymbol{E}_H = (\ln \lambda_i)\, \boldsymbol{M}_i \otimes \boldsymbol{M}_i = \ln \boldsymbol{U}, \tag{3.23}$$

$$\boldsymbol{E} = \frac{1}{2}(\lambda_i^2 - 1)\, \boldsymbol{M}_i \otimes \boldsymbol{M}_i = \frac{1}{2}\left(\boldsymbol{U}^2 - \boldsymbol{I}\right) = \frac{1}{2}\left(\boldsymbol{F}^T \boldsymbol{F} - \boldsymbol{I}\right) \ . \tag{3.24}$$

$\boldsymbol{E}_B$ is the Biot (extensional) strain tensor. It is the most intuitive strain measure. Its main disadvantage is that it cannot be directly expressed in terms of the deformation gradient $\boldsymbol{F}$, but rather has to be calculated from it by a polar decomposition. $\boldsymbol{E}_H$ is the Hencky (logarithmic)

strain (which is also not expressible in terms of $\boldsymbol{F}$ alone). Its one-dimensional form, Eq. (3.20), clearly demonstrates that $d\boldsymbol{E}_H$ is an incremental strain that measures incremental changes in the length of material line elements relative to their *current* length. Finally, $\boldsymbol{E}$ is the Green-Lagrange (metric) strain. While it is difficult to motivate its one-dimensional form, Eq. (3.21), its tensorial form has a clear physical meaning. To see this, consider infinitesimal line elements of size $d\ell$ and $d\ell'$ in the reference and deformed configurations respectively and construct the following measure of the change in their length

$$(d\ell')^2 - (d\ell)^2 = dx_i dx_i - dX_i dX_i = F_{ij} dX_j F_{ik} dX_k - dX_j \delta_{jk} dX_k = \tag{3.25}$$
$$2dX_j \left[\frac{1}{2} \left(F_{ij} F_{ik} - \delta_{jk} \right) \right] dX_k = 2dX_j \left[\frac{1}{2} \left(F_{ji}^T F_{ik} - \delta_{jk} \right) \right] dX_k \equiv 2dX_j E_{jk} dX_k \ .$$

Therefore,

$$\boldsymbol{E} = \frac{1}{2} \left(\boldsymbol{F}^T \boldsymbol{F} - \boldsymbol{I} \right) = \frac{1}{2} \left(\boldsymbol{C} - \boldsymbol{I} \right) = \frac{1}{2} \left(\boldsymbol{U}^2 - \boldsymbol{I} \right) = \frac{1}{2} (\boldsymbol{H} + \boldsymbol{H}^T + \boldsymbol{H}^T \boldsymbol{H}) \ , \tag{3.26}$$

where $\boldsymbol{C} \equiv \boldsymbol{F}^T \boldsymbol{F}$ is the right Cauchy-Green deformation tensor. So $\boldsymbol{E}$ is indeed a *material* metric strain tensor. Further note that $\boldsymbol{E}$ is quadratically nonlinear in the displacement gradient $\boldsymbol{H}$. The linear part of $\boldsymbol{E}$

$$\boldsymbol{\varepsilon} \equiv \frac{1}{2} (\boldsymbol{H} + \boldsymbol{H}^T) \tag{3.27}$$

is the linear (infinitesimal) strain tensor, which is not a true strain measure (as it is *not* rotationally invariant), but nevertheless is the basic object in the linearized field theory of elasticity (to be discussed later in the course). We can easily derive the *spatial* counterpart of $\boldsymbol{E}$, by having $(d\ell')^2 - (d\ell)^2 \equiv 2dx_j e_{jk} dx_k$, with (prove)

$$\boldsymbol{e} = \frac{1}{2} \left(\boldsymbol{I} - \boldsymbol{F}^{-T} \boldsymbol{F}^{-1} \right) = \frac{1}{2} \left(\boldsymbol{I} - \boldsymbol{b}^{-1} \right) \ . \tag{3.28}$$

$\boldsymbol{b} \equiv \boldsymbol{F} \boldsymbol{F}^T$ is the left Cauchy-Green deformation tensor (also termed the Finger tensor, which is sometimes denoted by $\boldsymbol{B}$). $\boldsymbol{e}$, known as the Euler-Almansi strain tensor, is a *spatial* metric strain tensor.

The deformation gradient $\boldsymbol{F}$ maps objects from the undeformed to the deformed configuration. For example, consider a volume element in the deformed configuration (assume $\boldsymbol{F}$ has already been diagonalized)

$$d\boldsymbol{x}^3 = dx_1 dx_2 dx_3 = F_{11} dX_1 F_{22} dX_2 F_{33} dX_3 = J(\boldsymbol{X}, t) d\boldsymbol{X}^3 \ , \tag{3.29}$$

where

$$J(\boldsymbol{X}, t) = \det \boldsymbol{F}(\boldsymbol{X}, t) \ . \tag{3.30}$$

Consider then a surface element in the undeformed configuration $d\boldsymbol{S} = dS\,\boldsymbol{N}$, where dS an infinitesimal area and $\boldsymbol{N}$ is a unit normal. The corresponding surface element in the deformed configuration is $d\boldsymbol{s} = ds\,\boldsymbol{n}$. To relate these quantities, we consider an arbitrary line element $d\boldsymbol{X}$ going through $d\boldsymbol{S}$ and express the spanned volume element by a dot product $d\boldsymbol{X}^3 = d\boldsymbol{S} \cdot d\boldsymbol{X}$. $d\boldsymbol{X}$ maps to $d\boldsymbol{x}$, which spans a corresponding volume element in the deformed configuration $d\boldsymbol{x}^3 = d\boldsymbol{s} \cdot d\boldsymbol{x}$. Using Eq. (3.29), the relation $d\boldsymbol{s} \cdot \boldsymbol{F} d\boldsymbol{X} = \boldsymbol{F}^T d\boldsymbol{s} \cdot d\boldsymbol{X}$ (i.e. $ds_i F_{ij} dX_j = F_{ji}^T ds_i dX_j$) and the fact that $d\boldsymbol{X}$ is an arbitrary line element, we obtain

$$d\boldsymbol{S} = J^{-1}\boldsymbol{F}^T d\boldsymbol{s} \ . \tag{3.31}$$

The spatial velocity gradient $\boldsymbol{L}(\boldsymbol{x}, t)$ is defined as

$$\boldsymbol{L} \equiv \frac{\partial \boldsymbol{v}(\boldsymbol{x}, t)}{\partial \boldsymbol{x}} = \dot{\boldsymbol{F}} \boldsymbol{F}^{-1} \ . \tag{3.32}$$

The symmetric part of $\boldsymbol{L}$, $\boldsymbol{D} = \frac{1}{2}(\boldsymbol{L} + \boldsymbol{L}^T)$, is an important quantity called the *rate of deformation* tensor. The anti-symmetric part of $\boldsymbol{L}$, $\boldsymbol{W} = \frac{1}{2}(\boldsymbol{L} - \boldsymbol{L}^T)$, is called the *spin (vorticity)* tensor.

B. The concept of stress

As was mentioned at the beginning of this section, material deformation is induced by forces. In order to describe and quantify forces at the continuum level we need the concept of *stress* (sketched earlier in section II to motivate the need for tensors). Consider a surface element $d\boldsymbol{s}$ in the deformed configuration. It is characterized by an outward normal $\boldsymbol{n}$ and a unit area ds. The surface element can be a part of the external boundary of the body or a part of an imaginary internal surface. The force acting on it, either by external agents in the former case or by neighboring material in the latter case, is denoted by $d\boldsymbol{f}$. We postulate, following Cauchy, that we can define a *traction vector* $\boldsymbol{t}$ such that

$$d\boldsymbol{f} = \boldsymbol{t}(\boldsymbol{x}, t, \boldsymbol{n})\, ds \ . \tag{3.33}$$

Cauchy proved that there exists a unique symmetric second-order tensor $\boldsymbol{\sigma}(\boldsymbol{x}, t)$ (i.e. $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$, the physical meaning of which will be discussed later) such that

$$\boldsymbol{t}(\boldsymbol{x}, t, \boldsymbol{n}) = \boldsymbol{\sigma}(\boldsymbol{x}, t)\, \boldsymbol{n} \ . \tag{3.34}$$

The spatial tensor $\boldsymbol{\sigma}$ is called the *Cauchy stress*. Its physical meaning becomes clear when we write Eq. (3.34) in components form, $t_i = \sigma_{ij} n_j$. Therefore, σ_{ij} is the force per unit area in the

ith direction, acting on a surface element whose outward normal has a component n_j in the jth direction. A corollary of Eq. (3.34)

$$t(\boldsymbol{x},t,-\boldsymbol{n}) = -t(\boldsymbol{x},t,\boldsymbol{n}) \ , \tag{3.35}$$

is nothing but *Newton's third law (action and reaction).*

As $\boldsymbol{\sigma}$ is defined in terms of the deformed configuration, which is not known a priori (one should solve for it using the stresses themselves), $\boldsymbol{\sigma}$ is not always a useful quantity (it is the only relevant quantity in the linearized field theory of elasticity, where we do not distinguish between the deformed and undeformed configurations). To overcome this difficulty, we can define alternative stress measures that are useful for calculations. In general, we will show later that thermodynamics allows us to define for any strain measure a work-conjugate stress measure. Here, we define one such mechanically-motivated stress measure. Let us define a (fictitious) reference configuration traction vector $\boldsymbol{T}(\boldsymbol{X},t,\boldsymbol{N})$ as

$$d\boldsymbol{f} = t(\boldsymbol{x},t,\boldsymbol{n})\,ds = \boldsymbol{T}(\boldsymbol{X},t,\boldsymbol{N})\,dS \ , \tag{3.36}$$

where $\boldsymbol{N}$ and dS are the reference outward normal and unit area, respectively, whose images in the deformed configuration are $\boldsymbol{n}$ and ds, respectively. Following Cauchy, there exists a tensor $\boldsymbol{P}(\boldsymbol{X},t)$ such that

$$\boldsymbol{T}(\boldsymbol{X},t,\boldsymbol{N}) = \boldsymbol{P}(\boldsymbol{X},t)\,\boldsymbol{N} \ . \tag{3.37}$$

$\boldsymbol{P}(\boldsymbol{X},t)$ is called the *first Piola-Kirchhoff stress tensor.* In fact, it is not a true tensor (it relates quantities from the deformed and undeformed configuration and hence, like $\boldsymbol{F}$, is a two-point tensor) and is not symmetric. Using the above properties, it is straightforward to show that it is related to the Cauchy stress $\boldsymbol{\sigma}$ by

$$\boldsymbol{P} = J\boldsymbol{\sigma}\boldsymbol{F}^{-T} \ . \tag{3.38}$$

The concepts of strain and stress will allow us to formulate physical laws, such as conservation laws and the laws of thermodynamics, and constitutive laws which describe material behaviors, in the rest of this course.

IV. EQUATIONS OF MOTION, THE LAWS OF THERMODYNAMICS AND OBJECTIVITY

A. Conservation laws

We first consider the mass density in the reference configuration $\rho_0(\boldsymbol{X}, t)$. The conservation of mass simply implies that

$$M = \int_{\Omega_0} \rho_0(\boldsymbol{X}, t) d\boldsymbol{X}^3 \tag{4.1}$$

is time-independent (Ω_0 is the region occupied by the body in the reference configuration), i.e.

$$\frac{DM}{Dt} = \frac{D}{Dt} \int_{\Omega_0} \rho_0(\boldsymbol{X}, t) d\boldsymbol{X}^3 = \frac{D}{Dt} \int_{\Omega} \rho(\boldsymbol{x}, t) d\boldsymbol{x}^3 = 0 \ , \tag{4.2}$$

where Ω is the region occupied by the body in the deformed configuration. The integral form can be easily transformed into a local form. In the reference (Lagrangian) configuration it simply reads

$$\frac{D\rho_0}{Dt} = \frac{\partial \rho_0(\boldsymbol{X}, t)}{\partial t} = 0 \quad \Longrightarrow \quad \rho_0(\boldsymbol{X}, t) = \rho_0(\boldsymbol{X}) \ . \tag{4.3}$$

To obtain the local form in the Eulerian description, note that (by the definition of J, cf. Eq. (3.29)) $\rho_0(\boldsymbol{X}) = \rho(\boldsymbol{x}, t) J(\boldsymbol{X}, t)$ and $\dot{J} = J \nabla_{\boldsymbol{x}} \cdot \boldsymbol{v}$ (prove). Therefore,

$$\frac{D\rho_0}{Dt} = \frac{D}{Dt} \Big[\rho(\boldsymbol{x}, t) J(\boldsymbol{X}, t) \Big] = J \frac{D\rho}{Dt} + J\rho \nabla_{\boldsymbol{x}} \cdot \boldsymbol{v} = 0 \ , \tag{4.4}$$

which implies

$$\frac{D\rho(\boldsymbol{x}, t)}{Dt} + \rho(\boldsymbol{x}, t) \nabla_{\boldsymbol{x}} \cdot \boldsymbol{v}(\boldsymbol{x}, t) = \frac{\partial \rho(\boldsymbol{x}, t)}{\partial t} + \nabla_{\boldsymbol{x}} \cdot \Big(\rho(\boldsymbol{x}, t) \boldsymbol{v}(\boldsymbol{x}, t) \Big) = 0 \ . \tag{4.5}$$

This expression of local mass conservation (continuity equation) takes the general form of a local conservation law

$$\frac{\partial(\text{field})}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\text{field flux}) = \text{source} \ . \tag{4.6}$$

Let us now discuss a theorem that will be very useful in formulating and manipulating other conservation laws. Consider the following 1D integral

$$I(t) = \int_{\varphi(X_1, t)}^{\varphi(X_2, t)} \psi(x, t) dx \ . \tag{4.7}$$

Note that $X_{1,2}$ are fixed here. Taking the time derivative of $I(t)$ (Leibnitz's rule) we obtain

$$\dot{I}(t) = \int_{\varphi(X_1, t)}^{\varphi(X_2, t)} \partial_t \psi(x, t) dx + \psi \Big(\varphi(X_2, t), t \Big) \partial_t \varphi(X_2, t) - \psi \Big(\varphi(X_1, t), t \Big) \partial_t \varphi(X_1, t) \ . \tag{4.8}$$

First recall that (generally in 3D)

$$V(X, t) = \partial_t \varphi(X, t) = v(x, t) \ . \tag{4.9}$$

Then note that since X_1 and X_2 are fixed in the integral we can interpret the time derivative as a material time derivative D/Dt. Therefore, we can rewrite Eq. (4.8) as

$$\frac{D}{Dt} \int_{\varphi(X_1, t)}^{\varphi(X_2, t)} \psi(x, t) dx = \int_{\varphi(X_1, t)}^{\varphi(X_2, t)} \left[\partial_t \psi(x, t) + \partial_x \Big(\psi(x, t) v(x, t) \Big) \right] dx \ . \tag{4.10}$$

The immediate generalization of this result to volume integrals over a time dependent domain Ω reads

$$\frac{D}{Dt} \int_\Omega \psi(x, t) dx^3 = \int_\Omega \left[\partial_t \psi(x, t) + \nabla_x \cdot \Big(\psi(x, t) v(x, t) \Big) \right] dx^3 \ . \tag{4.11}$$

This is the Reynolds' transport theorem which is very useful in the context of formulating conservation laws. This is the same Osborne Reynolds (1842-1912), who is known for his studies of the transition from laminar to turbulent fluid flows, and who gave the Reynolds number its name.

Using mass conservation, we obtain (prove)

$$\frac{D}{Dt} \int_\Omega \rho(x, t) \psi(x, t) dx^3 = \int_\Omega \rho(x, t) \frac{D\psi(x, t)}{Dt} dx^3 \ . \tag{4.12}$$

This is very useful when we choose $\psi(x, t)$ to be a quantity per unit mass. In particular, setting $\psi = 1$ we recover the conservation of mass.

Linear momentum balance (Newton's second law) reads

$$\dot{P}(t) = \frac{D}{Dt} \int_{\Omega_0} \rho_0(X) V(X, t) dX^3 = \frac{D}{Dt} \int_\Omega \rho(x, t) v(x, t) dx^3 = F(t) \ , \tag{4.13}$$

where $F(t)$ is the total force acting on a volume element Ω (do not confuse P with the first Piola-Kirchhoff stress tensor of Eq. (3.37)). To obtain a local form of this law note that the total force is obtained by integrating local tractions (surface forces) $t(x, t)$ and body (volume) forces $b(x, t)$, i.e.

$$F(t) = \int_{\partial\Omega} t(x, t, n) ds + \int_\Omega b(x, t) dx^3 \ , \tag{4.14}$$

where $\partial\Omega$ is the boundary of the volume element. Use Cauchy's stress theorem of Eq. (3.34) and the divergence (Gauss) theorem of Eq. (2.27) to obtain

$$\int_{\partial\Omega} t(x, t, n) ds = \int_{\partial\Omega} \sigma(x, t) n ds = \int_\Omega \nabla_x \cdot \sigma(x, t) dx^3 \ . \tag{4.15}$$

Use then Reynold's transport theorem of Eq. (4.12), with ψ replaced by the spatial velocity field v, to transform the linear momentum balance of Eq. (4.13) into

$$\int_\Omega \left[\nabla_x \cdot \sigma(x, t) + b(x, t) - \rho(x, t) \dot{v}(x, t) \right] dx^3 = 0 \ . \tag{4.16}$$

Since this result is valid for an arbitrary material volume, we obtain the following spatial (Eulerian) local form of linear momentum conservation

$$\nabla_{\boldsymbol{x}} \cdot \boldsymbol{\sigma} + \boldsymbol{b} = \rho\, \dot{\boldsymbol{v}} = \rho\left(\partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} \boldsymbol{v}\right) \ . \tag{4.17}$$

Note that this equation does not conform with the structure of a general conservation law in Eq. (4.6). This can be achieved (prove), yielding

$$\frac{\partial(\rho\, \boldsymbol{v})}{\partial t} - \nabla_{\boldsymbol{x}} \cdot \left(\rho\, \boldsymbol{v} \otimes \boldsymbol{v} - \boldsymbol{\sigma}\right) = \boldsymbol{b} \ . \tag{4.18}$$

A similar analysis can be developed for the angular momentum. However, the requirement that the angular acceleration remains finite implies that angular momentum balance, at the continuum level, is satisfied if the Cauchy stress tensor $\boldsymbol{\sigma}$ is symmetric, i.e.

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T \ , \tag{4.19}$$

to be derived in the tutorial. We note that the symmetry of the Cauchy stress tensor emerges from the conservation of angular momentum if the continuum assumption is valid at all lengthscales. Real materials, however, may possess intrinsic lengthscales associated with their microstructure (e.g. grains, fibers and cellular structures). In this case, we need generalized theories which endow each material point with translational and rotational degrees of freedom, describing the displacement and rotation of the underlying microstructure. One such theory is known as Cosserat (micropolar) continuum, which is a continuous collection of particles that behave like rigid bodies. Under such circumstances one should consider a couple-stress tensor (which has the dimensions of stress × length) as well, write down an explicit angular momentum balance equation and recall that the ordinary stress tensor is no longer symmetric.

The local momentum conservation laws can be expressed in Lagrangian forms. For example, the linear momentum balance, Eq. (4.17), translates into (prove)

$$\nabla_{\boldsymbol{X}} \cdot \boldsymbol{P} + \boldsymbol{B} = \rho_0 \dot{\boldsymbol{V}} \ , \tag{4.20}$$

where $\boldsymbol{P}$ is the first Piola-Kirchhoff stress tensor of Eq. (3.37) and $\boldsymbol{B}(\boldsymbol{X},t) = J(\boldsymbol{X},t)\boldsymbol{b}(\boldsymbol{x},t)$. This equation is extremely useful because it allows calculations to be done in a fixed undeformed coordinate system $\boldsymbol{X}$. It is important to note that one should also transform the boundary conditions of a given problem from the deformed configuration (where they are physically imposed) to the underformed configuration.

B.   The laws of thermodynamics

Equilibrium thermodynamics is a well-established branch of physics, whose modern incarnation is deeply rooted in statistical mechanics. This framework, known as statistical thermodynamics, builds on systematic coarse-graining of statistical descriptions of microscopic dynamics. It gives rise to an effective macroscopic description of large physical systems through a small set of state variables. In the spirit of this course, we do not follow the microscopic route of statistical mechanics (a topic covered in complementary courses), but rather focus on a macroscopic perspective.

Let us consider the balance of mechanical energy (thermal energy is excluded here and will be discussed soon). The external mechanical power $\mathcal{P}_{ext}$ is simply the rate at which mechanical work is being done by external forces, either boundary traction $\boldsymbol{t}$ or body forces $\boldsymbol{b}$. It reads

$$\mathcal{P}_{ext} = \int_{\partial\Omega} \boldsymbol{t} \cdot \boldsymbol{v} ds + \int_{\Omega} \boldsymbol{b} \cdot \boldsymbol{v} d\boldsymbol{x}^3 \ . \tag{4.21}$$

The external mechanical work is transformed into kinetic energy $\mathcal{K}$ and internal mechanical power $\mathcal{P}_{int}$. These are expressed as

$$\mathcal{K} = \int_{\Omega} \frac{1}{2} \rho \boldsymbol{v}^2 \, d\boldsymbol{x}^3 \tag{4.22}$$

and

$$\mathcal{P}_{int} = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{L} \, d\boldsymbol{x}^3 = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{D} \, d\boldsymbol{x}^3 \ . \tag{4.23}$$

Therefore, mechanical energy balance reads

$$\mathcal{P}_{ext} = \mathcal{P}_{int} + \dot{\mathcal{K}} \ . \tag{4.24}$$

It can be easily proven using Eqs. (4.17) and (4.21).

To arrive at the first law of thermodynamics we need to consider another form of energy — thermal energy. This form of energy accounts for the random (microscopic) motion of particles, which was excluded from the previous discussion. To properly describe this form of energy we need two concepts, that of an internal energy $\mathcal{U}$ and that of thermal power $\mathcal{Q}$. The internal energy accounts for all microscopic forms of energy. Here we focus on mechanical and thermal energies, but in general electric, magnetic, chemical and other forms of energy can be included. $\mathcal{U}$ can be associated with a density u (per unit mass) and hence

$$\mathcal{U} = \int_{\Omega} \rho(\boldsymbol{x}, t) \, u(\boldsymbol{x}, t) \, d\boldsymbol{x}^3 \ . \tag{4.25}$$

Note that the total energy is the sum of kinetic and internal energies $\mathcal{K} + \mathcal{U}$. The thermal (heat) power $\mathcal{Q}$ is expressed, as usual, in terms of fluxes and sources

$$\mathcal{Q} = -\int_{\partial\Omega} \boldsymbol{q}\cdot\boldsymbol{n}\, ds + \int_{\Omega} r\, d\boldsymbol{x}^3 \ . \tag{4.26}$$

$\boldsymbol{q}$ is the heat flux and r is a (volumetric) heat source (e.g. radiation). For simplicity we exclude r from the discussion below. Finally, we note that the rate of change of internal energy is the sum of rate of change of internal mechanical energy and thermal power

$$\dot{\mathcal{U}} = \mathcal{P}_{int} + \mathcal{Q} \ , \tag{4.27}$$

which can be regarded as a statement of *the first law of thermodynamics*. Alternatively, by eliminating $\mathcal{P}_{int}$ between Eqs. (4.24) and (4.27) we obtain

$$\dot{\mathcal{K}} + \dot{\mathcal{U}} = \mathcal{P}_{ext} + \mathcal{Q} \ , \tag{4.28}$$

which is yet another statement of the same law. It has a clear physical meaning: external mechanical work and heat supply are transformed into kinetic and internal energies. An important point to note is that this law only tells us that one form of energy can be transformed into another form, but does not tell us anything about the direction of such processes. This global law can be readily transformed into a local form (prove), which reads

$$\rho\,\dot{u} = \boldsymbol{\sigma}:\boldsymbol{D} - \nabla_{\boldsymbol{x}}\cdot\boldsymbol{q} \ . \tag{4.29}$$

It is well known that many physical processes feature a well-defined direction, e.g. heat flows from a higher temperature to a lower one. This is captured by the second law of thermodynamics. To formulate the law we need two additional concepts, entropy and temperature. The total entropy $\mathcal{S}$ is a measure of microscopic "disorder" and is well defined in the framework of statistical mechanics. The absolute temperature T (a non-negative scalar), which is also a well defined statistical mechanical concept, is introduced such that the entropy increase associated with a thermal power $\mathcal{Q}$ is $\mathcal{Q}/T$. The second law then reads

$$\dot{\mathcal{S}} \geq -\int_{\partial\Omega} \frac{\boldsymbol{q}\cdot\boldsymbol{n}}{T}\, ds + \int_{\Omega} \frac{r}{T}\, d\boldsymbol{x}^3 = \frac{\mathcal{Q}}{T} \ , \tag{4.30}$$

where the last equality is valid for space-independent T (otherwise, T is part of the integrands and one cannot globally separate the heat power $\mathcal{Q}$ and the temperature T in the second law). The inequality in (4.30) states that the increase in the entropy of a system is larger than (or

equals to) the influx of entropy by heat (thermal power). When the system under consideration is closed (e.g. the universe) the second law states that the entropy is an increasing function of time (or constant), i.e. $\dot{\mathcal{S}} \geq 0$. Note that sometimes the entropy production rate Σ is defined as $\Sigma = \dot{\mathcal{S}} - \dot{\mathcal{Q}}/T$, which is non-negative.

Every macroscopic physical system, and consequently every theory of such systems, cannot violate the non-negativity of the entropy production rate Σ. This is a serious and very useful constraint on developing continuum theories of non-equilibrium phenomena. Yet, applying the second law constraint to arbitrarily far from equilibrium phenomena is not trivial (e.g. it might raise questions about the validity of the entropy concept itself) and will be further discussed later in the course.

The most well-developed application, however, of the second law constraint emerges in the context of *Linear Response Theory* describing systems that deviate only slightly from equilibrium (i.e. when driving forces are weak). In this case, the entropy production rate Σ can be expressed as a bilinear form in the deviation from equilibrium, defining a set of linear response coefficients. These linear response coefficients must satisfy various constraints to ensure consistency with the second law of thermodynamics. In fact, by invoking microscopic time reversibility Lars Onsager showed that these coefficients possess additional symmetries that go beyond the second law of thermodynamics, known as Onsager's reciprocal relations. The Nobel Prize in Chemistry in 1968 was awarded to Onsager for this fundamental contribution (the prize citation referred to "the discovery of the reciprocal relations bearing his name, which are fundamental for the thermo-dynamics of irreversible processes"). It is worth mentioning in the context of linear irreversible thermodynamics that Prigogine showed in 1945 that Onsager's reciprocal relations imply that the entropy production rate Σ attains a minimum under non-equilibrium steady-state conditions (which was one of the major reasons for awarding him the Nobel prize in 1977). Prigogine's principle of minimum entropy production generated considerable excitement at the beginning, but later on it was realized that this result (like Onsager's reciprocal relations) is specific to small deviations from equilibrium (linear response).

Let us consider a simple example of the implications of the second law of thermodynamics for an isolated system that is composed of two subsystems of different temperatures $T_1 > T_2$. The subsystems are separated by a wall that allows heat transport, but not mass or mechanical work transport. Since the system as a whole is isolated and no mechanical work is involved, the first

and second laws of thermodynamics read

$$\dot{\mathcal{S}} = \dot{\mathcal{S}}_1 + \dot{\mathcal{S}}_2 \geq 0 \quad \text{and} \quad \dot{\mathcal{U}} = \dot{\mathcal{U}}_1 + \dot{\mathcal{U}}_2 = 0 \ . \tag{4.31}$$

While heat cannot flow into the system from the outer world, heat can possibly flow through the wall separating the two subsystems, the rate of which is denoted as $\mathcal{Q}_{1\to2}$. We assume that the entropy and energy changes of each subsystem is a result of the heat transfer across the wall, i.e.

$$\dot{\mathcal{S}}_1 = -\frac{\mathcal{Q}_{1\to2}}{T_1} = \frac{\dot{\mathcal{U}}_1}{T_1} \quad \text{and} \quad \dot{\mathcal{S}}_2 = \frac{\mathcal{Q}_{1\to2}}{T_2} = \frac{\dot{\mathcal{U}}_2}{T_2} \ . \tag{4.32}$$

Substituting this in the second law we obtain

$$\dot{\mathcal{S}} = \mathcal{Q}_{1\to2} \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \geq 0 \ , \tag{4.33}$$

which can be satisfied by

$$\mathcal{Q}_{1\to2} = A(T_1 - T_2) \quad \text{with} \quad A \geq 0 \tag{4.34}$$

to leading order in the temperature difference (resulting in Newton's cooling law). Therefore, heat flows from a higher temperature to a lower one.

To obtain a local version of the second law define an entropy density $s(\boldsymbol{x}, t)$ (per unit mass) such that

$$\mathcal{S} = \int_\Omega \rho(\boldsymbol{x}, t)\, s(\boldsymbol{x}, t)\, d\boldsymbol{x}^3 \ , \tag{4.35}$$

which immediately leads to (recall Eq. (4.30))

$$\rho\, \dot{s} + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{q}/T) \geq 0 \ . \tag{4.36}$$

Eliminating $\nabla_{\boldsymbol{x}} \cdot \boldsymbol{q}$ between the first and second laws in Eqs. (4.29) and (4.36) we obtain

$$\boldsymbol{\sigma} : \boldsymbol{D} - \rho\, \dot{u} + T\rho\, \dot{s} - \frac{\boldsymbol{q} \cdot \nabla_{\boldsymbol{x}} T}{T} \geq 0 \ . \tag{4.37}$$

Usually this inequality is split into two stronger inequalities

$$\boldsymbol{\sigma} : \boldsymbol{D} - \rho\, \dot{u} + T\rho\, \dot{s} \geq 0 \quad \text{and} \quad \boldsymbol{q} \cdot \nabla_{\boldsymbol{x}} T \leq 0 \ . \tag{4.38}$$

The second inequality is satisfied by choosing

$$\boldsymbol{q} = -\kappa \nabla_{\boldsymbol{x}} T \ , \tag{4.39}$$

where $\kappa \geq 0$ is the thermal conductivity. This is Fourier's law of heat conduction. The first inequality in (4.38) is known as the dissipation inequality (or the Clausius-Planck inequality) and

will play an important role later in the course. Any physical theory must satisfy this inequality. We note that the dissipation inequality can be also expressed in terms of the Helmholtz free-energy density $f = u - Ts$ (per unit mass) as

$$\boldsymbol{\sigma} : \boldsymbol{D} - \rho \dot{f} - \rho s \dot{T} \geq 0 \ . \tag{4.40}$$

Under isothermal conditions, $\dot{T} = 0$, we have

$$\boldsymbol{\sigma} : \boldsymbol{D} - \rho \dot{f} \geq 0 \ . \tag{4.41}$$

C. Heat equations

Heat equations are manifestations of the first law of thermodynamic. To see this, substitute Fourier's law of Eq. (4.39) into the first law of Eq. (4.29) to obtain

$$\rho \dot{u} = \boldsymbol{\sigma} : \boldsymbol{D} + \kappa \nabla_{\boldsymbol{x}}^2 T \ . \tag{4.42}$$

This equation is transformed into a heat equation once we consider a constitutive law (see below) for the rate of deformation $\boldsymbol{D}$ and the internal energy density u. In the simplest case, which you know very well, we consider a non-deforming body $\boldsymbol{D} = 0$ such that the local internal energy changes only due to heat flow. Therefore, we define the specific heat capacity through $c\dot{T} \equiv \rho \dot{u}$ and obtain

$$\dot{T} = D \nabla_{\boldsymbol{x}}^2 T \ , \tag{4.43}$$

where here $D \equiv \kappa/c$ is the thermal diffusion coefficient (the ratio of thermal conductivity and the specific heat capacity). This is just the ordinary heat diffusion equation, which in fact remains valid also for elastically deforming materials. Later in the course we will encounter more general heat equations that emerge in the present of more complicated constitutive laws.

A small digression

Diffusion equations possess an interesting feature, which is not always appreciated and which will teach us an important lesson about continuum physics. The modern microscopic theory of diffusion (and Brownian motion) is one of the most well-understood problems in physics and one of the greatest successes of statistical mechanics. To make things as simple and concrete as possible, we focus here on particle diffusion in 1d. Within this theory, diffusion is described by a particle

which makes a random walk along the x-axis, starting at $x=0$ when the clock is set to $t=0$. At each time interval $\Delta t=1$ (in this discussion all quantities are dimensionless) the particle makes a jump of size $|\Delta x|=1$ to the right or the left, with equal probability. Statistical mechanics tells us (through the central limit theorem) that after a sufficiently long period of time (i.e. number of jumps), the probability distribution function $p(x,t)$ reads

$$p(x,t) = \frac{e^{-\frac{x^2}{2t}}}{\sqrt{2\pi t}} \, , \tag{4.44}$$

i.e. a normal distribution with zero mean and variance which is just the time t. This continuous probability distribution function is the solution of a diffusion equation of the form

$$\partial_t p(x,t) = \frac{1}{2}\partial_{xx}p(x,t) \, , \tag{4.45}$$

which is a 1d version of Eq. (4.43) (with $D=1/2$ and recall that it is dimensionless here), with the initial condition

$$p(x,t=0) = \delta(x) \, . \tag{4.46}$$

This appears to be a strong result of continuum physics where we describe a physical system on timescales and lengthscales much larger than atomistic, forgetting about the discreteness of matter (think of this equation as describing the time evolution of an ink droplet spreading inside a water tank, where p represents for the mass density of the ink). Is there actually a problem here? Well, there is. Eq. (4.44) tells us that at time t after the initiation of the process, when the probability was localized at $x=0$ (cf. Eq. (4.46)), there is a *finite* probability to find the particle (e.g. an ink molecule) at an *arbitrarily large* x. The fact that this probability is exponentially small is beside the point. The crucial observation is that it is non-zero, implying that information propagated from $x = 0$ (at $t = 0$) *infinitely* fast. This violates fundamental physics (causality, relativity theory or whatever).

On the other hand, we know from the microscopic description of the problem that

$$p(x,t) = 0 \quad \text{for} \quad |x| > t \, , \tag{4.47}$$

i.e. that at most the particle could have made all of the jumps in one direction. That means that in fact the probability propagates at a finite speed (in our dimensionless units the propagation speed is 1), as we expect from general considerations.

So what went wrong in the transition from the microscopic description to macroscopic one? The answer is that Eq. (4.44) is wrong when $|x|$ becomes significantly larger than $\mathcal{O}(\sqrt{t})$. A more

careful microscopic analysis (not discussed here) actually gives rise to the following continuum evolution equation for $p(x,t)$

$$\partial_t p(x,t) + \frac{1}{2}\partial_{tt} p(x,t) = \frac{1}{2}\partial_{xx} p(x,t) \ , \tag{4.48}$$

which is a combination of a wave equation and a diffusion equation. The fastest propagation of probability is limited by ordinary wave propagation of speed 1, exactly as we expect from microscopic considerations. This equation reconciles the apparent contradiction discussed above, showing that both Eqs. (4.44) and (4.47) are valid, just on different ranges of x for a given time t. This shows that the continuum limit should be taken carefully and critically. Beware. And you can also relax, the diffusion equation is in fact a very good approximation in most physical situations of interest.

We note that Eq. (4.48) is another equation of continuum physics, known as the telegrapher's equation. It was originally derived in a completely different context, that of electric transmission lines with losses, by Oliver Heaviside (1850-1925). This is the guy who invented the Heaviside step function and formulated Maxwell's equations using vector calculus in the form known to us today (the original ones were much uglier). He also independently discovered the Poynting vector (which is named after John Henry Poynting).

As noted above, the telegrapher's equation in Eq. (4.48) contains in it a 1d scalar wave equation (here for the probability distribution function $p(x,t)$). We will soon see that in the context of reversible deformation, and when higher dimensions are considered, the tensorial nature of deformation implies even more interesting and richer wave equations, and associated phenomena. Stay tuned.

D. Objectivity (frame‑indifference)

To conclude this part of the course we consider the important notion of objectivity or frame-indifference. To quantify this idea we consider two observers that move (rotationally and translationally) one with respect to the other. For simplicity we assume that their watches are synchronized and that at time $t=0$ they agree on the reference configuration $\boldsymbol{X}$ of the body under consideration. The motions observed by the two observers are related by the following change-of-observer transformation

$$\boldsymbol{\varphi}^*(\boldsymbol{X},t) = \boldsymbol{Q}(t)\boldsymbol{\varphi}(\boldsymbol{X},t) + \boldsymbol{y}(t) \ , \tag{4.49}$$

where $\boldsymbol{Q}(t)$ is a proper time-dependent rotation matrix

$$\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I} \quad \text{and} \quad \det(\boldsymbol{Q}) = +1 \tag{4.50}$$

and $\boldsymbol{y}(t)$ is a time-dependent translation vector. A scalar ψ is classified as objective (frame-indifferent) if it satisfies $\psi^* = \psi$. A *spatial* vector $\boldsymbol{u}$ is objective if $\boldsymbol{u}^* = \boldsymbol{Q}\boldsymbol{u}$ and a *spatial* tensor $\boldsymbol{a}$ is objective if $\boldsymbol{a}^* = \boldsymbol{Q}\boldsymbol{a}\boldsymbol{Q}^T$ (we will try, for notational consistency, to denote spatial tensor by lowercase symbols). *Material/Lagrangian* objective vectors and tensors remain unchanged under change-of-observer transformation. Hybrid quantities, such as two-point tensors (which have a mixed spatial-material nature), have other objectivity criteria (see below).

To see how this works, consider the spatial velocity field $\boldsymbol{v} = \partial_t \boldsymbol{\varphi}$. Then we have

$$\boldsymbol{v}^* = \partial_t \boldsymbol{\varphi}^* = \boldsymbol{Q}\partial_t \boldsymbol{\varphi} + \dot{\boldsymbol{Q}}\boldsymbol{\varphi} + \dot{\boldsymbol{y}} = \boldsymbol{Q}\boldsymbol{v} + \dot{\boldsymbol{Q}}\boldsymbol{\varphi} + \dot{\boldsymbol{y}} \ . \tag{4.51}$$

Therefore, the velocity field is in general not objective. It can be made objective if we restrict ourselves to time-independent rigid transformation in which $\dot{\boldsymbol{Q}} = \dot{\boldsymbol{y}} = 0$. Likewise, the spatial acceleration field $\boldsymbol{a} = \dot{\boldsymbol{v}}$ is not an objective vector. This means that the linear momentum balance equation (i.e. Newton's second law) is not objective under the transformation in Eq. (4.49). This happens because time-dependent $\boldsymbol{Q}(t)$ and $\boldsymbol{y}(t)$ generate additional forces (centrifugal, Coriolis etc.). This is well-known to us: classical physics is invariant only under Galilean transformations, i.e. when $\dot{\boldsymbol{Q}} = 0$ and $\ddot{\boldsymbol{y}} = 0$. The classical laws of nature are the same in all inertial frames (and we know how to account for forces that emerge in non-inertial frames).

The important point to note is that for constitutive laws, i.e. physical laws that describe material behaviors, people sometimes demand something stronger: they insist that these laws remain unchanged under the change-of-observer transformation of Eq. (4.49) for general $\boldsymbol{Q}(t)$ and $\boldsymbol{y}(t)$. That is, even though Newton's second law is objective only under Galilean transformations, one usually demands constitutive laws to be objective under a more general transformation. This is called "The principle of material frame-indifference". To see how this works, consider then the deformation tensor $\boldsymbol{F}$. We have

$$\boldsymbol{F}^* = \nabla_{\boldsymbol{X}}\boldsymbol{\varphi}^*(\boldsymbol{X},t) = \boldsymbol{Q}\nabla_{\boldsymbol{X}}\boldsymbol{\varphi}(\boldsymbol{X},t) = \boldsymbol{Q}\boldsymbol{F} \ . \tag{4.52}$$

Therefore, $\boldsymbol{F}$ does not transform like an objective tensor, but rather like an objective vector. This is because it is not a true tensor, but rather a two-point tensor (a tensor that connects two spaces, $\boldsymbol{X}$ and $\boldsymbol{x}$ in this case). Two-point tensors (i.e. tensors of mixed spatial-material nature), that

satisfy $\boldsymbol{A}^* = \boldsymbol{Q}\boldsymbol{A}$ under a change-of-observer transformation, are regarded as objective. Hence, $\boldsymbol{F}$ is regarded as an objective two-point tensor.

To see the difference between *material* and *spatial* objective tensors, consider the right Cauchy-Green deformation tensor $\boldsymbol{C}$ (see Eq. (3.26)) and the left Cauchy-Green deformation (Finger) tensor $\boldsymbol{b}$ (see Eq. (3.28)). For the former, we have

$$\boldsymbol{C}^* = \boldsymbol{F}^{*T}\boldsymbol{F}^* = \boldsymbol{F}^T\boldsymbol{Q}^T\boldsymbol{Q}\boldsymbol{F} = \boldsymbol{F}^T\boldsymbol{F} = \boldsymbol{C} \ , \tag{4.53}$$

i.e. $\boldsymbol{C}$ is an objective material tensor. For the latter, we have

$$\boldsymbol{b}^* = \boldsymbol{F}^*\boldsymbol{F}^{*T} = \boldsymbol{Q}\boldsymbol{F}\boldsymbol{F}^T\boldsymbol{Q}^T = \boldsymbol{Q}\boldsymbol{b}\boldsymbol{Q}^T \ , \tag{4.54}$$

i.e. $\boldsymbol{b}$ is an objective spatial tensor.

The Cauchy stress $\boldsymbol{\sigma}$ is an objective tensor, i.e. $\boldsymbol{\sigma}^* = \boldsymbol{Q}\boldsymbol{\sigma}\boldsymbol{Q}^T$. This can be easily shown by using Eq. (3.34), $\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n}$, and by noting that both $\boldsymbol{t}$ and $\boldsymbol{n}$ are objective vectors. Consider then the velocity gradient, $\boldsymbol{L} = \partial\boldsymbol{v}/\partial\boldsymbol{x} = \dot{\boldsymbol{F}}\boldsymbol{F}^{-1}$, for which we have

$$\boldsymbol{L}^*\boldsymbol{F}^* = \dot{\boldsymbol{F}}^* \implies \boldsymbol{L}^*\boldsymbol{Q}\boldsymbol{F} = \boldsymbol{Q}\dot{\boldsymbol{F}} + \dot{\boldsymbol{Q}}\boldsymbol{F} \implies \boldsymbol{L}^* = \boldsymbol{Q}\boldsymbol{L}\boldsymbol{Q}^T + \dot{\boldsymbol{Q}}\boldsymbol{Q}^T \ . \tag{4.55}$$

Therefore, $\boldsymbol{L}$ is not an objective tensor and hence if one adopts "The principle of material frame-indifference" then $\boldsymbol{L}$ cannot be used to formulate physical laws. However, by noting that $\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}$ implies $\dot{\boldsymbol{Q}}\boldsymbol{Q}^T = -\boldsymbol{Q}\dot{\boldsymbol{Q}}^T$, we immediately conclude that the rate of deformation tensor $\boldsymbol{D}$ is objective. Many physical theories involve the time rate of change of a tensor, for example a stress rate. However, it is immediately observed that $\dot{\boldsymbol{\sigma}}$ is not an objective tensor. To see this, note that Eq. (4.55) implies $\dot{\boldsymbol{Q}}\boldsymbol{Q}^T = \boldsymbol{W}^* - \boldsymbol{Q}\boldsymbol{W}\boldsymbol{Q}^T \implies \dot{\boldsymbol{Q}} = \boldsymbol{W}^*\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{W}$ and write

$$\begin{aligned}
\dot{\boldsymbol{\sigma}}^* &= \dot{\boldsymbol{Q}}\boldsymbol{\sigma}\boldsymbol{Q}^T + \boldsymbol{Q}\dot{\boldsymbol{\sigma}}\boldsymbol{Q}^T + \boldsymbol{Q}\boldsymbol{\sigma}\dot{\boldsymbol{Q}}^T \\
&= \left(\boldsymbol{W}^*\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{W}\right)\boldsymbol{\sigma}\boldsymbol{Q}^T + \boldsymbol{Q}\dot{\boldsymbol{\sigma}}\boldsymbol{Q}^T + \boldsymbol{Q}\boldsymbol{\sigma}\left(\boldsymbol{Q}^T\boldsymbol{W}^{*T} - \boldsymbol{W}^T\boldsymbol{Q}^T\right) \\
&= \boldsymbol{W}^*\boldsymbol{\sigma}^* + \boldsymbol{\sigma}^*\boldsymbol{W}^{*T} + \boldsymbol{Q}\left(\dot{\boldsymbol{\sigma}} - \boldsymbol{W}\boldsymbol{\sigma} - \boldsymbol{\sigma}\boldsymbol{W}^T\right)\boldsymbol{Q}^T \ .
\end{aligned} \tag{4.56}$$

Use now $\boldsymbol{W}^T = -\boldsymbol{W}$ to rewrite the last relation as

$$\dot{\boldsymbol{\sigma}}^* + \boldsymbol{\sigma}^*\boldsymbol{W}^* - \boldsymbol{W}^*\boldsymbol{\sigma}^* = \boldsymbol{Q}\left(\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{W} - \boldsymbol{W}\boldsymbol{\sigma}\right)\boldsymbol{Q}^T \ , \tag{4.57}$$

or equivalently as

$$\dot{\boldsymbol{\sigma}}^* + [\boldsymbol{\sigma}^*, \boldsymbol{W}^*] = \boldsymbol{Q}\left(\dot{\boldsymbol{\sigma}} + [\boldsymbol{\sigma}, \boldsymbol{W}]\right)\boldsymbol{Q}^T \ , \tag{4.58}$$

where $[\cdot]$ is the commutator of two tensors. This result shows that indeed $\dot{\boldsymbol{\sigma}}$ is not an objective tensor, but also suggests that

$$\overset{\triangle}{\boldsymbol{\sigma}} \equiv \dot{\boldsymbol{\sigma}} + [\boldsymbol{\sigma}, \boldsymbol{W}] \tag{4.59}$$

is an objective stress rate tensor. This derivative is called Jaumann derivative and is extensively used in solid mechanics. It is important to note that there is **no** unique way to define an objective tensorial time derivative, and in fact there are infinitely many others (some of which are rather common). The Jaumann derivative, as well as other objective stress rates, can be used to formulate physical theories.

What is the basic status of objectivity? Is it a fundamental principle of classical physics or is it just a very useful approximation (that, by definition, has limitations)? Since macroscopic constitutive laws should ultimately result from systematic coarse-graining of microscopic physics, and since the latter obviously satisfy Newton's second law, there must exist situations in which objectivity is violated. In particular, in situations in which centrifugal and Coriolis forces cannot be neglected at the molecular level, objectivity cannot be fully satisfied. On the other hand, in many situations this is a very useful approximation that allows us to further constrain the structure of constitutive laws. So we must conclude that objectivity cannot be a "principle" of physics, rather an approximation (possibly a very useful/fruitful one).

While objectivity is widely invoked, its basic status has been the subject of many heated debates. An example from the 1980's can be found at: Physical Review A **32**, 1239 (1985), and the subsequent comment and reply. See also some insightful comments made by de Gennes, Physica A **118**, 43 (1983).

Constitutive laws

Up to now we considered measures of deformation and the concept of stress, conservation laws, the laws of thermodynamics and symmetry principles. These are not enough to describe the behavior of materials. The missing piece is a physical theory for the response of the material to external forces, the so-called constitutive relations/laws. To see the mathematical necessity of constitutive laws, consider the momentum balance equations of (4.17) in 2D, in the quasi-static limit (no inertia) and neglecting body forces

$$\partial_x \sigma_{xx} + \partial_y \sigma_{xy} = 0 \quad \text{and} \quad \partial_x \sigma_{yx} + \partial_y \sigma_{yy} = 0 \ . \tag{4.60}$$

These are two equations for 3 fields. Additional information about how stresses are related to the state of deformation of a body is required.

In the rest of the course we will consider physical theories for the behavior of materials. These must be consistent with the laws of thermodynamics discussed above and to comply with the principle of objectivity (frame-indifference, in its either weak or strong form). While thermodynamics, objectivity and symmetry principles seriously limit and constrain physical theories and are very useful, to understand material behaviors we need additional physical input.

Reversible processes: non-dissipative constitutive behaviors

The simplest response of a solid to mechanical driving forces is elastic. By elastic we mean that the response is reversible, i.e. that when the driving forces are removed the system relaxes back to its original state. Put in other words, elasticity means that the system "remembers" its undeformed state, which can serve as a reference configuration. Later in the course we will discuss irreversible deformation processes in which the internal state of a physical system evolves, and no recovery of the original state is observed when external constraints are removed. When an elastic system is deformed, energy is being stored in it. Suppose that the deformation is described by the Green-Lagrange strain measure $\boldsymbol{E}$, cf. Eq. (3.26), then the elastic energy density is described by the functional $u(\boldsymbol{E}, s)$. All of the physics of elasticity is encapsulated in this strain-energy functional.

V. THE LINEARIZED FIELD THEORY OF ELASTICITY

A. General derivation for anisotropic and isotropic materials

In many situations solids deform only slightly within the range of relevant driving forces. Think, for example, about your teeth when you eat a nut or about all metal objects around you. This is true for "hard" solids. However, things are different when we consider "soft" solids like rubbers (e.g. your car tire), gels or various biological materials (e.g. your skin). While they also deform elastically, they require a finite deformation description, as will be explained later in the course.

If the deformation remains small, we can focus on situations in which the displacement gradient is small $|\boldsymbol{H}| \ll 1$ (in fact we also require small rotations, see below). Under these conditions, we can linearize the Green-Lagrange strain $\boldsymbol{E} \simeq \boldsymbol{\varepsilon} = \frac{1}{2}(\boldsymbol{H} + \boldsymbol{H}^T)$, cf. Eq. (3.27), and use only the infinitesimal strain tensor $\boldsymbol{\varepsilon}$. This will make our life much easier (but please do not relax, it will be still quite tough nonetheless). But there is a price; first, as we already discussed, $\boldsymbol{\varepsilon}$ is **not** rotationally invariant. A corollary of this lack of rotational invariance is that a constitutive law formulated in terms of $\boldsymbol{\varepsilon}$ will not be objective. To see this, note that

$$\boldsymbol{E}^* = \frac{1}{2}\left(\boldsymbol{C}^* - \boldsymbol{I}\right) = \frac{1}{2}\left(\boldsymbol{C} - \boldsymbol{I}\right) = \boldsymbol{E} \ . \tag{5.1}$$

That is, $\boldsymbol{E}$ is an objective material tensor, which immediately implies that $\boldsymbol{\varepsilon}$ is not. So already in our first discussion of a constitutive relation we violate objectivity. We can easily adhere to it formally, but the practical price will be high as it will force us to go nonlinear. In a *huge* range of problems, though, rotations remain small and $\boldsymbol{\varepsilon}$ does a remarkable job in properly describing the relevant physics.

Another great advantage of the linearity assumption is that we should no longer distinguish between the undeformed $\boldsymbol{X}$ and deformed $\boldsymbol{x}$ configurations. The reason is that while these configurations are of course distinct in the presence of deformation, and as the displacements themselves can be large the difference can be large itself, gradients remain small and all physical quantities are indistinguishable to linear order. Moreover, the convective term in the material derivative plays no role as it is intrinsically nonlinear. The linearized strain tensor takes the form

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{5.2}$$

and we can also identify $\boldsymbol{D}$ with $\dot{\boldsymbol{\varepsilon}}$. Finally, since in the context of the linearized theory of elasticity mass density variations are small (the mass density appears only as a multiplicative

factor in products and hence effectively contributes only to higher orders), we can use quantities per unit volume rather than quantities per unit mass. In particular, we define $\rho\, u \equiv \bar{u}$ and $\rho\, s \equiv \bar{s}$, and for the ease of notation drop the bars.

Under these conditions, the dissipation inequality of the second law of thermodynamics of Eq. (4.38) reads $\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{u} + T\,\dot{s} \geq 0$. To proceed, we express $\dot{u}(\boldsymbol{\varepsilon}, s)$ in terms of variations in $\boldsymbol{\varepsilon}$ and s and substitute in the above inequality to get

$$\left(\boldsymbol{\sigma} - \frac{\partial u}{\partial \boldsymbol{\varepsilon}}\right) : \dot{\boldsymbol{\varepsilon}} + \left(T - \frac{\partial u}{\partial s}\right)\dot{s} \geq 0 \ . \tag{5.3}$$

Since elastic response is reversible, we expect an equality to hold. Moreover, the strain and the entropy can be varied independently. Therefore, the second law analysis implies

$$\boldsymbol{\sigma} = \frac{\partial u}{\partial \boldsymbol{\varepsilon}} \quad \text{and} \quad T = \frac{\partial u}{\partial s} \ . \tag{5.4}$$

There is a related, more formal, approach to derive these relations. We focus on (5.3), without assuming an equality. However, we do note that u and $\boldsymbol{\sigma}$ are independent of $\dot{\boldsymbol{\varepsilon}}$. That is a basic property of an elastic response: the rate at which a state is reached makes no difference. Therefore, the only way to avoid violating the inequality under all circumstances is to set the brackets to zero (the same argument holds for the entropy term). This is termed the Coleman-Noll procedure.

The resulting relations are thermodynamic identities that are derived from the second law of thermodynamics. The first one says that the stress $\boldsymbol{\sigma}$ is thermodynamically conjugate to the strain $\boldsymbol{\varepsilon}$. The strain energy functional takes the form (we assume that the entropy does not change with deformation and hence is irrelevant here)

$$u = \frac{1}{2}\,\sigma_{ij}\,\varepsilon_{ij} \ , \tag{5.5}$$

where linearity implies a tensorial linear relation between the stress and the strain $\boldsymbol{\sigma} = \boldsymbol{C}\boldsymbol{\varepsilon}$ (also explaining the appearance of $1/2$ in the expression above for the strain energy density) or in components

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \ . \tag{5.6}$$

The response coefficients, C_{ijkl}, known as the elastic constants (the forth order tensor $\boldsymbol{C}$ is known as the stiffness tensor), are given by

$$C_{ijkl} = \frac{\partial^2 u}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \ . \tag{5.7}$$

Equation (5.6) is a constitutive relation, i.e. a relation between the stress (driving force) and the strain (response), which is a generalization of Hooke's relation for an elastic spring ($F = -k\,x$).

How many independent numbers are needed to describe $\boldsymbol{C}$? Naively, one would think that $3^4 = 81$ independent numbers are needed. However, $\boldsymbol{C}$ possesses various general symmetries that significantly reduce the amount of independent numbers, even before considering any specific material symmetries. First, the symmetry of the Cauchy stress tensor implies, through Eq. (5.6), that

$$C_{ijkl} = C_{jikl} . \tag{5.8}$$

Furthermore, the symmetry of the infinitesimal strain tensor, $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^T$, implies

$$C_{ijkl} = C_{ijlk} . \tag{5.9}$$

These two symmetries imply that we need only 36 independent numbers (6 for the first two indices and 6 for the last two). Furthermore, since $\boldsymbol{C}$ is obtained through a second-order tensorial derivative of the energy density u, see Eq. (5.7), interchanging the order of differentiation suggests an additional symmetry of the form

$$C_{ijkl} = C_{klij} . \tag{5.10}$$

The latter imposes 15 additional constraints ($\frac{6 \times 5}{2}$), which leaves us with 21 independent numbers. Therefore, in the most general case $\boldsymbol{C}$ contains 21 independent elastic coefficients (in fact, $\boldsymbol{C}$ can be represented as a 6 by 6 symmetric matrix — which depends on 21 independent numbers —, where the components of $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are represented as vectors with 6 components).

This is the extreme anisotropic case. However, usually materials exhibit some symmetries that further reduce the number of independent elastic constants. For example, composite materials (e.g. fiberglass, a glass-fiber reinforced plastic) may be invariant with respect to various translations and rotations. Here we focus on isotropic materials. Since the energy functional is a scalar, it depends only on invariants of $\boldsymbol{\varepsilon}$, which can be written as $\operatorname{tr} \boldsymbol{\varepsilon}$, $\operatorname{tr} \boldsymbol{\varepsilon}^2$ and $\operatorname{tr} \boldsymbol{\varepsilon}^3$ (sometimes people use other invariants that are linearly dependent on these). Since in a linear theory the energy must be quadratic in the strain, only two combinations, $(\operatorname{tr} \boldsymbol{\varepsilon})^2$ and $\operatorname{tr} \boldsymbol{\varepsilon}^2$, can appear and hence

$$u(\boldsymbol{\varepsilon}) = \frac{\lambda}{2}(\operatorname{tr} \boldsymbol{\varepsilon})^2 + \mu \operatorname{tr} \boldsymbol{\varepsilon}^2 . \tag{5.11}$$

It is important to note that we can replace $\boldsymbol{\varepsilon}$ by $\boldsymbol{E}$ in this energy functional to obtain the *simplest* possible nonlinear elastic material model

$$u(\boldsymbol{E}) = \frac{\lambda}{2}(\operatorname{tr} \boldsymbol{E})^2 + \mu \operatorname{tr} \boldsymbol{E}^2 . \tag{5.12}$$

This constitutive law, termed the Saint Venant-Kirchhoff material model, is both rotationally invariant and objective. Alas, it is also nonlinear due to the inherent geometric nonlinearity in

$\boldsymbol{E}$. This constitutive law is the simplest nonlinear elastic model because it is *constitutively* linear, i.e. $u(\boldsymbol{E})$ is quadratic in $\boldsymbol{E}$, but is *geometrically* nonlinear (due to the nonlinear dependence of $\boldsymbol{E}$ on $\boldsymbol{H}$). Here we adhere to a constitutive law which is linear in $\boldsymbol{H}$, and hence use Eq. (5.11).

Equation (5.11) shows that isotropic linear elastic materials are characterized by only two elastic constants, the Lamé constants. μ is also known as the shear modulus (can we say something about the sign of λ and μ at this stage?). Using the following differential tensorial relation

$$\frac{d \operatorname{tr}\boldsymbol{A}^n}{d\boldsymbol{A}} = n(\boldsymbol{A}^{n-1})^T \ , \tag{5.13}$$

the constitutive law (Hooke's law) can be readily obtained

$$\boldsymbol{\sigma} = \lambda \operatorname{tr}\boldsymbol{\varepsilon}\,\boldsymbol{I} + 2\mu\,\boldsymbol{\varepsilon} \tag{5.14}$$

or in components

$$\sigma_{ij} = \lambda\varepsilon_{kk}\,\delta_{ij} + 2\mu\,\varepsilon_{ij} \ . \tag{5.15}$$

The stiffness tensor can be written as $C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. It is important to stress that Hooke's law is simply a perturbation theory based on a gradient expansion. This is entirely analogous to the constitutive law for Newtonian fluids, which is based on a velocity gradient expansion (μ in Hooke's law plays the role of shear viscosity and λ the role of bulk viscosity).

Let us first consider a few homogeneous deformation situations. Consider a solid that is strained uniaxially (say in the x-direction) by an amount $\varepsilon_{xx} = \varepsilon$. The stress state of the solid is described by $\sigma_{xx} = \sigma$ and all of the other components vanish (because the lateral boundaries are free). Symmetry implies that the strain response is $\varepsilon_{ij} = 0$ for $i \neq j$ and $\varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_\perp$. Our goal is to calculate the response σ and $\varepsilon_\perp$ in terms of the driving ε. Using Eq. (5.15) we obtain

$$0 = \lambda(\varepsilon + 2\varepsilon_\perp) + 2\mu\varepsilon_\perp \quad \text{and} \quad \sigma = \lambda(\varepsilon + 2\varepsilon_\perp) + 2\mu\varepsilon \ . \tag{5.16}$$

Solving for the response functions $\sigma(\varepsilon)$ and $\varepsilon_\perp(\varepsilon)$ we obtain

$$\varepsilon_\perp = -\frac{\lambda}{2(\lambda + \mu)}\varepsilon \equiv -\nu\,\varepsilon \quad \text{and} \quad \sigma = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}\varepsilon \equiv E\,\varepsilon \ . \tag{5.17}$$

E is known as Young's modulus and ν as Poisson's ratio. These response coefficients are most easily measured experimentally and are therefore extensively used. In many cases, Hooke's law is expressed in terms of them (derive). The latter analysis immediately tells us something about ν in a certain limit.

Let us then consider an isotropic compression of a solid. In this case we have $\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = -p$, where p is the hydrostatic pressure, and $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon$ (all other components of the stress and strain tensors vanish). We then have

$$-p = \frac{3\lambda + 2\mu}{3} \operatorname{tr}\boldsymbol{\varepsilon} \equiv K \operatorname{tr}\boldsymbol{\varepsilon} . \tag{5.18}$$

Noting that the relative change in volume is given by $\delta V/V = \det \boldsymbol{F} - 1 = (1 + \epsilon_{xx})(1 + \epsilon_{yy})(1 + \epsilon_{zz}) - 1 \simeq \operatorname{tr}\boldsymbol{\varepsilon}$, we see that K is the bulk modulus, which we are already familiar with from thermodynamics, $K = -V\partial p/\partial V$. Using the bulk modulus we can express the energy functional of Eq. (5.11) as

$$u(\boldsymbol{\varepsilon}) = \frac{1}{2}K(\operatorname{tr}\boldsymbol{\varepsilon})^2 + \mu \left(\varepsilon_{ij} - \frac{1}{3}\operatorname{tr}\boldsymbol{\varepsilon}\,\delta_{ij} \right)^2 . \tag{5.19}$$

The components in the second brackets are the components of the deviatoric strain tensor, $\boldsymbol{\varepsilon}^{dev} \equiv \boldsymbol{\varepsilon} - \frac{1}{3}\operatorname{tr}\boldsymbol{\varepsilon}\,I$, where $\operatorname{tr}\boldsymbol{\varepsilon}^{dev} = 0$. The representation in Eq. (5.19) shows that the total strain energy can be associated with a deviatoric (shear-like) part, weighted by the shear modulus μ, and a volumetric (dilatational) part, weighted by the bulk modulus K. Another important implication of this representation is that μ and K multiply terms which are positive definite and independently variable. The importance of this observation is that thermodynamics implies that at (stable) equilibrium the (free) energy attains a minimum and hence u must be positive under all circumstances. Since the deformation can be either volume conserving, $\operatorname{tr}\boldsymbol{\varepsilon} = 0$, or isotropic, $\boldsymbol{\varepsilon} \propto \boldsymbol{I}$, we must have

$$\mu, K > 0 . \tag{5.20}$$

This has interesting implications for other elastic constants. For example, it tells us that $\lambda \geq -2\mu/3$, which shows that λ is not necessarily positive. Taking the two extreme cases, $\lambda = -2\mu/3$ and $\lambda \gg \mu$, we obtain the following constraint on Poisson's ratio

$$-1 \leq \nu \leq \frac{1}{2} . \tag{5.21}$$

Therefore, while a negative ν might appear counterintuitive (as it implies that a solid expands in the directions orthogonal to the uniaxial stretch direction), it does not violate any law of physics. An example for a natural material with a Poisson's ratio of nearly zero is cork, used as a stopper for wine bottles.

In the last few decades there has been an enormous interest in materials with unusual values of Poisson's ratio. In particular, materials with a negative Poisson's ratio were synthesized (they are termed auxetic materials), see the review article in Nature Materials, "Poisson's ratio and

modern materials", Nature Materials 10, 823–837 (2011) (see http://www.nature.com/nmat/journal/v10/n11/pdf/nmat3134.pdf). You may also want to look at: http://silver.neep.wisc.edu/~lakes/Poisson.html. Such materials are a subset of a larger class of materials known as "Metamaterials". Metamaterials are artificial materials designed to provide properties which may not be readily available in nature, and can be very interesting and useful.

The power and limitations of the continuum assumption can be nicely illustrated through a discussion of the evolution of the concept of Poisson's ratio, from Poisson's original paper in 1827, which based on the molecular hypothesis, through the subsequent development based on the competing continuum hypothesis, to the explosion of research in this direction in recent decades based on a better microscopic/mesoscopic understanding of the structure of materials and computational capabilities.

The upper bound of ν also have a clear physical meaning. In a uniaxial test we have

$$\operatorname{tr}\boldsymbol{\varepsilon} = (1 - 2\nu)\varepsilon \, , \tag{5.22}$$

which immediately tells us that incompressible materials, i.e. materials for which $\operatorname{tr}\boldsymbol{\varepsilon} = 0$, have $\nu = 1/2$. In fact, the incompressibility limit is a bit subtle. To see this, recall Eq. (5.18), $-p = K \operatorname{tr}\boldsymbol{\varepsilon}$. Obviously, a finite pressure can be applied to an incompressible material. This means that in the incompressibility limit we have $\operatorname{tr}\boldsymbol{\varepsilon} \to 0$ and $K \to \infty$, while their product is finite. It is also clear that no work is invested in applying a pressure to an incompressible material and no energy is being stored. Indeed, in the incompressibility limit we have $K(\operatorname{tr}\boldsymbol{\varepsilon})^2 \to 0$. Note also that while $K \propto (1 - 2\nu)^{-1}$ diverges in the incompressibility limit, the shear modulus μ and Young's modulus E remain finite. Finally, we stress that the bounds on Poisson's ratio in Eq. (5.21) are valid for *isotropic* materials. *Anisotropic* materials can, and actually do, violate these bounds.

Before we move on to derive the equations of motion for a linear elastic solid, we note a few properties of the linearized (infinitesimal) strain tensor $\boldsymbol{\varepsilon}$. First, as we stressed several times above, it is not invariant under finite rotations (prove). That means that even if the relative distance change between material points remains small, $\boldsymbol{\varepsilon}$ cannot be used when rotations are not small. In that sense it is not a true strain measure. Second, the components of $\boldsymbol{\varepsilon}$ are not independent. The reason for this is that $\boldsymbol{\varepsilon}$ is derived from a continuously differentiable displacement field $\boldsymbol{u}$. The resulting relations between the different components of $\boldsymbol{\varepsilon}$, ensuring that the different parts of a material fit together after deformation, are termed "compatibility conditions". In 3D there are 6 such conditions, making a problem formulated in terms of strain components very complicated,

and in 2D there is only one compatibility condition, which reads

$$\partial_{yy}\varepsilon_{xx} + \partial_{xx}\varepsilon_{yy} = 2\partial_{xy}\varepsilon_{xy} \ . \tag{5.23}$$

Finally, note that compatibility is automatically satisfied if the displacement field is used directly.

The equation of motion describing linear elastic solids is readily obtained by substituting the constitutive relation (Hooke's law) of Eq. (5.15) into the momentum balance equation of (4.17), taking the form

$$(\lambda + \mu)\nabla (\nabla \cdot \boldsymbol{u}) + \mu\nabla^2\boldsymbol{u} + \boldsymbol{b} = \rho\partial_{tt}\boldsymbol{u} \ . \tag{5.24}$$

It is called the Navier-Lamé equation. It accounts for a huge range of physical phenomena and can easily serve as the basis for a two-semester course. In spite of its linearity, its solutions in 3D and/or under dynamic situations might be very complicated and require (sometimes non-trivial) numerical methods.

There are, however, many situations in which analytical tools can be employed. One typical situation is when we are not interested in the exact solution, with all the π's 2's etc., but rather in the way the solution depends on the material's parameters, loading and geometry of a given problem. In this case we invoke everything we have at hand: physical considerations, symmetries, dimensional analysis etc. Let us demonstrate this in two examples (both are fully analytically tractable, but they will serve our purpose here).

Example: Surface Green's function

Consider a linear elastic, isotropic, half-space which is loaded at the flat surface by a concentrated force. We assume that the force is applied to an area which is small compared to the scales of interest (this will be a recurring theme later in the course), hence the pressure at the surface ($z = 0$) takes the form $p_z(x, y, z = 0) = F_z\delta(x)\delta(y)$, where the $x - y$ plane is parallel to the surface and z is perpendicular to it (note that $p_z = -\sigma_{zz}$). Focus then on the shape of the deformed (originally flat) surface, i.e. on $u_z(x, y, z = 0)$. What form can it take? First, the azimuthal symmetry of the force with respect to the surface, implies that u_z depends on x and y only through the radius r. Second, linearity implies that it must be proportional to F_z. Finally, since F_z has the dimension of force and u_z has the dimension of length, we need another quantity that involves force dimension. The only quantity available in the problem is the elastic modulus

E (or μ). Put all these ingredients together, we must have

$$u_z(r, z=0) \sim \frac{F_z}{E\,r} \ . \tag{5.25}$$

This gives us the shape of the deformed surface. Note that since there is no lengthscale in the problem, the shape is scale-free. Of course the singularity at $r \to 0$ is not physical, it simply means that as we approach the applied force the details of how it is applied, as well as material nonlinearities, matter and actually regularize the singularity. If we compare our result to the exact one we discover that we indeed only missed a prefactor of order unity, which takes the form $(1-\nu^2)/\pi$. Since we have considered a concentrated force, our result is valid for any surface pressure distribution, i.e. we have a calculated a Green's function. Therefore, for a general surface pressure distribution $p_z(x, y, z = 0)$, we have

$$u_z(x, y, z=0) = \frac{1 - \nu^2}{\pi\,E} \int \frac{p_z(x', y', z = 0)dx'dy'}{\sqrt{(x - x')^2 + (y - y')^2}} \ . \tag{5.26}$$

Example: Hertzian contact

Consider a linear elastic sphere of radius R that is pressed against an infinitely rigid plane by a force F. This problem was considered (and solved) by Hertz in 1882 and is known as the Hertzian contact problem (in fact, Hertz considered two deforming spheres). It signaled the birth of contact mechanics and is of enormous importance and range of applications. These span the full range from friction and tribology of small structures, through earthquakes in the earth crust to rubble piles in the solar system. In order to get the essence of Hertz's solution without actually solving the partial differential equations we need a physical insight, a geometrical insight and a constitutive relation. Denote the distance by which the sphere approaches the plane by δ and the radius of the circular contact that is formed by a. The crucial physical question to ask (and to answer, of course) is what the typical lengthscale of the strain distribution is. Since strains are built in the sphere only because of the formed contact, we expect the strain distribution to be concentrated on a scale a (where the rest of the sphere responds essentially in a rigid body manner). Therefore, the displacement δ is accumulated on a scale a near the surface and the typical strain is

$$\varepsilon \sim \frac{\delta}{a} \ . \tag{5.27}$$

This is the physical insight we needed. The geometrical observation is simple and reads

$$a^2 \sim \delta R \ , \tag{5.28}$$

i.e. for a given displacement δ the contact area is linear in the sphere's radius R (to see this simply cut from the bottom of a sphere of radius R a piece of height δ and estimate the cut area). Note also that the last equation implies that $a \ll R$ since δ is small. Using the constitutive relation, Hooke's law, we have

$$p_0 \sim \frac{F}{a^2} \sim E\varepsilon \sim \frac{E\,\delta}{a} \quad \Rightarrow \quad F \sim E\delta a \, , \tag{5.29}$$

where p_0 is a typical pressure. Using the last two equations, we can calculate the 3 relevant "response" functions $a(F; R, E)$, $\delta(F; R, E)$ and $p_0(F; R, E)$ to be

$$a \sim \left(\frac{FR}{E}\right)^{1/3} , \quad \delta \sim \left(\frac{F^2}{R\,E^2}\right)^{1/3} , \quad p_0 \sim \left(\frac{FE^2}{R^2}\right)^{1/3} . \tag{5.30}$$

Therefore, we managed to express the response quantities in terms of the driving force (F), geometry (R) and constitutive parameters (E). These players (i.e. the driving forces, geometry and constitutive relations) are generic players in our game. Comparing the resulting expressions above to the exact ones indeed shows that they are correct to within numerical constants of order unity. These results are rather striking. How come a linear theory gave rise to a nonlinear response, i.e. a nonlinear dependence of the response quantities on the driving force F? The answer is that nonlinearities were hidden in the geometry of the problem. In other words, the fact that the contact area is a variable that depends self-consistently on the deformation, but is unknown a priori, makes the problem effectively nonlinear. Contact problems are highly nonlinear even within the framework of a linear elastic field theory. As a final comment, we note that p_0 represents the pressure at the center of the contact. The pressure must drop to zero at the contact line, $r = a$ (r is measured from the center). The result (not derived here) reads

$$p(r, z=0) = p_0 \sqrt{1 - \frac{r^2}{a^2}} \, , \tag{5.31}$$

where $z=0$ is the location of the rigid plane. This shows that while the pressure is continuous at the contact line, its derivative is not.

Before we consider further simplifications of the Navier-Lamé equation of (5.24), let us explore some of their general properties. For that purpose, recall the identity $\nabla^2 \boldsymbol{u} = \nabla(\nabla \cdot \boldsymbol{u}) - \nabla \times (\nabla \times \boldsymbol{u})$. Applying it to the Navier-Lamé Eq. (5.24), in the absence of body forces $(\boldsymbol{b} = 0)$ and under equilibrium (static) conditions (no inertia), we obtain

$$(\lambda + 2\mu)\nabla (\nabla \cdot \boldsymbol{u}) - \mu \nabla \times (\nabla \times \boldsymbol{u}) = 0 \, . \tag{5.32}$$

Acting with the divergence operator on this equation, we obtain

$$\nabla^2 (\nabla \cdot \boldsymbol{u}) = 0 \ , \tag{5.33}$$

since $\nabla \cdot (\nabla \times \boldsymbol{A}) = 0$ for any vector field $\boldsymbol{A}$. This shows that under equilibrium (static) conditions $\nabla \cdot \boldsymbol{u}$ satisfies Laplace's equation, i.e. it is harmonic. Operating then with the Laplacian operator on the Navier-Lamé Eq. (5.24), we obtain

$$\nabla^2 \nabla^2 \boldsymbol{u} = 0 \ , \tag{5.34}$$

i.e. under equilibrium (static) conditions $\boldsymbol{u}$ satisfies bi-Laplace's equation, i.e. it is a bi-harmonic vector field. These results are useful in various contexts.

B. 2D Elasticity

We now turn to discuss further simplifications of the Navier-Lamé Eq. (5.24). In many situations the dynamics of a linear elastic body can be approximated as two-dimensional.

1. Scalar elasticity

The simplest possible such situation is when the only non-vanishing component of the displacement field is given by $u_z(x, y, t)$. This physical situation is termed anti-plane deformation. In this case, the Navier-Lamé Eq. (5.24) reduces to

$$\mu \nabla^2 u_z = \rho \partial_{tt} u_z \ , \tag{5.35}$$

which is a scalar wave equation. $c_s = \sqrt{\mu/\rho}$ is the shear wave speed. Let us focus first on static situations in which this equation reduces to

$$\nabla^2 u_z = 0 \ , \tag{5.36}$$

i.e. u_z satisfies Laplace's equation (a harmonic function). Laplace's equation emerges in many branches of physics (electrostatics, fluid mechanics etc.). The theory of complex variable functions offers very powerful tools to solve 2D problems. We first discuss this approach for Laplace's equation in (5.36). Let us first briefly recall some fundamentals of complex functions theory. Let z be a complex variable, $z = x + iy$. A function $f(z)$ is called analytic if it satisfies

$$\partial_x f(z) = f'(z) \quad \text{and} \quad \partial_y f(z) = i f'(z) \ . \tag{5.37}$$

Writing $f(z)$ as $f(z) = u(x,y) + iv(x,y)$, Eq. (5.37) implies

$$f'(z) = \partial_x f(z) = \partial_x u + i\partial_x v = -i\partial_y f(z) = \partial_y v - i\partial_y u , \tag{5.38}$$

leading to the well-known Cauchy-Riemann conditions

$$\partial_x u = \partial_y v \quad \text{and} \quad \partial_x v = -\partial_y u . \tag{5.39}$$

Eq. (5.37) also implies the following operator relation

$$\partial_z = \frac{1}{2}(\partial_x - i\partial_y) . \tag{5.40}$$

Recalling that the complex conjugate of z is $\bar{z} = x - iy$, we also have

$$\partial_{\bar{z}} = \frac{1}{2}(\partial_x + i\partial_y) . \tag{5.41}$$

Any complex function $f(x,y)$ can be represented as $f(x,y) = g(z,\bar{z})$. Therefore, an analytic function is a function that is independent of $\bar{z}$. This observation immediately shows that *any* analytic function is a solution of Laplace's equation, e.g. the one in Eq. (5.36). To see this we note that

$$\nabla^2 = \partial_{xx} + \partial_{yy} = 4\partial_z\partial_{\bar{z}} . \tag{5.42}$$

Therefore,

$$u_z(x,y) = \Re[f(z)] \quad \text{or} \quad u_z(x,y) = \Im[f(z)] , \tag{5.43}$$

where $f(z)$ is sometimes called a complex potential (note the analogy with electric potential in electrostatics). Choosing the real or imaginary part is a matter of convenience. The specific solution $f(z)$ is selected so as to satisfy a specific set of boundary conditions. The stress tensor (in this case only the σ_{zx} and σ_{zy} components do not vanish) is given by (prove)

$$\sigma_{zy} + i\sigma_{zx} = \mu f'(z) , \tag{5.44}$$

when one chooses $u_z(x,y) = \Im[f(z)]$.

Example: Screw dislocations

Later in the course we will work out a more complicated example of how these powerful tools help us solving important problems. Here we would like to consider a simple example. For that aim we introduce an object called a "dislocation". Dislocations will appear later in the course as the

carriers of plastic deformation in crystalline and polycrystalline materials, and are very important and interesting objects. For our purposes here we define a dislocation as a continuum object that carries with it a topological charge and focus only on the static linear elastic consequences. By "topological charge" we mean that if we integrate the displacement field in a close loop around the dislocation core (where we define the origin of our coordinate system) we obtain a finite value, i.e.

$$\oint du_z = b \ . \tag{5.45}$$

This implies the existence of a branch cut. The magnitude of the topological charge, b, is the size of the so-called Burgers vector $\boldsymbol{b}$, $b = |\boldsymbol{b}|$ (named after the Dutch physicist Jan Burgers, who is also known for the famous fluid mechanics equation). In this case we have $\boldsymbol{b} = b\,\hat{z}$. Note that a dislocation is a line (and not a point) defect, which extends along the z-direction. Translation symmetry along this direction allows for a 2D treatment. Obviously, the generation of a dislocation is neither a linear process, nor an elastic one. Still, once it exists, we can ask ourselves what the linear elastic fields generated by the topological charge are. The field equation is (5.36) and the boundary condition is given by Eq. (5.45). The stress must vanish far away from the topological charge that generates it. As noted above, the boundary condition implies the existence of a branch cut. Linearity implies that $u_z \sim b$. We can meet all of these constraints and solve the field equation by choosing

$$u_z = \frac{b}{2\pi}\Im[\log z] = \frac{b\,\theta}{2\pi} \ . \tag{5.46}$$

Recall that $\log z = \log(re^{i\theta}) = \log r + i\theta$. This is a solution because $\log z$ has the proper branch cut, it is analytic outside the branch cut and it satisfies

$$\oint du_z = \frac{b}{2\pi} \int_{-\pi}^{\pi} d\theta = b \ . \tag{5.47}$$

Using Eq. (5.44) we obtain

$$\sigma_{zy} + i\sigma_{zx} = \frac{\mu b}{2\pi}\frac{x - iy}{x^2 + y^2} \sim \frac{\mu b}{r} \ . \tag{5.48}$$

Such a dislocation is known as a screw dislocation. As we said above, dislocations are very interesting objects. Here, by looking at the linear elastic consequences of dislocations, we already see one aspect of it. The linear elastic stress field diverges as $1/r$ near the core of a dislocation. The size of the Burgers vector b is atomic (typically a lattice spacing). The linear elastic solution is valid at distances larger than the dislocation core, whose size c is typically of the order of a few atomic spacings. The detailed structure of the topological defect within the core regularizes the linear elastic divergence. What happens at large distances? The stress (and strain) fields of

a dislocation decay very slowly in space, an observation that has profound consequences. To see this, let us calculate the energy of a single dislocation (per unit length in the z-direction)

$$U = \int u\, dx dy = \int_c^R \frac{1}{2}\sigma_{ij}\varepsilon_{ij} r dr d\theta \sim \mu b^2 \int_c^R \frac{rdr}{r^2} = \mu b^2 \log\left(\frac{R}{c}\right) , \qquad (5.49)$$

where R is the macroscopic size of the system. We see that the energy of a single dislocation diverges logarithmically with the size of the system. That means that when many dislocations are present (a number to bear in mind for a strongly deformed metal is $10^{15}\mathrm{m}^{-2}$), they are strongly interacting. Dislocations are amongst the most strongly interacting objects in nature. In addition, they are also amongst the most dissipative objects we know of, but that has to do with their motion, which we did not consider here.

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2.   Conformal invariance

</div>

Many equations of mathematical physics possess an important and very useful property called conformal invariance. A conformal transformation/mapping between the complex planes ω and z is defined as

$$z = \Phi(\omega) , \qquad (5.50)$$

where $\Phi(\omega)$ is an analytic function with a non-vanishing derivative, i.e. $\Phi'(\omega) \neq 0$. Conformal means (nearly literally) angle-preserving. To see this consider an infinitesimal line element in the ω-plane, $d\omega$, and its image in the z-plane, dz. They are related by

$$dz = \Phi'(\omega)d\omega . \qquad (5.51)$$

However,

$$\Phi'(\omega) = |\Phi'(\omega)|e^{i\arg[\Phi'(\omega)]} \qquad (5.52)$$

which means that every two infinitesimal line elements $d\omega$ going through the point ω_0 are mapped into their images dz going through $z_0 = \Phi(\omega_0)$ by a common expansion/contraction (determined by $|\Phi'(\omega_0)|$) and a common rotation (determined by the angle $\arg[\Phi'(\omega_0)]$). Therefore, the relative angle between them is preserved.

If a field equation is invariant under such a conformal transformation/mapping, then we can solve a given problem in a simple domain and immediately get the solution for a (more) complicated domain by a suitably chosen conformal transformation. This is a powerful mathematical tool. An example for a conformally invariant field equation is Laplace's equation in (5.36). To

show this we need to prove that any solution $f(z)$ of Laplace's equation in the z-plane remains a solution in the ω-plane under a conformal transformation $g(\omega) = f(\Phi(\omega))$. For this particular equation this is automatically satisfied since $g(\omega)$ is also an analytic function (because it is a composition of two harmonic functions). However, it would be useful to see how it works. First, note that we have

$$\partial_\omega f(\Phi(\omega)) = \Phi'(\omega)\partial_z f(z) \ , \tag{5.53}$$

i.e. $\partial_\omega = \Phi'(\omega)\partial_z$, which immediately implies $\partial_{\bar{\omega}} = \overline{\Phi'(\omega)}\partial_{\bar{z}}$. We then have

$$\partial_{\bar{\omega}}\partial_\omega f(\Phi(\omega)) = \partial_{\bar{\omega}}\left[\Phi'(\omega)\partial_z f(z)\right] =$$
$$\partial_z f(z)\partial_{\bar{\omega}}\Phi'(\omega) + \Phi'(\omega)\partial_{\bar{\omega}}\partial_z f(z) = |\Phi'(\omega)|^2\partial_{\bar{z}}\partial_z f(z) = 0 \ . \tag{5.54}$$

Therefore,

$$\partial_{\bar{\omega}}\partial_\omega f(\Phi(\omega)) = 0 \ , \tag{5.55}$$

which proves the conformal invariance of Laplace's equation. Later in the course we will use this result in the context of fracture mechanics. It is important to note that conformal invariance is a property of partial differential equations, not of differential operators. In the above example, the differential operator was not invariant, i.e. $\partial_{\bar{\omega}}\partial_\omega = |\Phi'(\omega)|^2\partial_{\bar{z}}\partial_z$, but the equation is. This, for instance, immediately implies that the Helmholtz equation, $\nabla^2 u + u = 0$ is not conformally invariant. Finally, recall that a differential equation is also defined by its boundary conditions, which should be conformally invariant as well. For Dirichlet ($u = $ const.) or Neumann ($\boldsymbol{n} \cdot \nabla u = 0$) boundary conditions this is satisfied, but other boundary conditions make things more complicated.

3. In-plane elasticity, Airy stress function

The Navier-Lamé Eq. (5.24) can be also reduced to 2D under in-plane deformation conditions. There are two possibilities here, one called "plane-stress" and the other one "plane-strain". To see how it is done, let us explicitly write Hooke's law in Eq. (5.15) in terms of E and ν. As was noted above, the stiffness tensor $\boldsymbol{C}$ in the relation $\boldsymbol{\sigma} = \boldsymbol{C}\boldsymbol{\varepsilon}$ can be represented as a 6 by 6 matrix

such that

$$
\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{zy} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-2\nu \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{zy} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{pmatrix} .
\tag{5.56}
$$

We can invert this relation into the form $\boldsymbol{\varepsilon} = \boldsymbol{S}\boldsymbol{\sigma}$, where $\boldsymbol{S} = \boldsymbol{C}^{-1}$ is the compliance tensor (if you noticed that $\boldsymbol{C}$ is called the stiffness tensor and $\boldsymbol{S}$ is called the compliance tensor and wondered about it, this is not a mistake and there is no intention to confuse you. It is a long-time convention that cannot be reverted anymore). We write the last relation explicitly as

$$
\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{zy} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{pmatrix} = \frac{1}{E} \begin{pmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1+\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1+\nu \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{zy} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix} .
\tag{5.57}
$$

We are now ready to perform the reduction to 2D.

Plane-stress

We first consider objects that are thin in one dimension, say z, and are deformed in the xy-plane. What happens in the z-direction? Since the two planes $z = 0$ and $z = h$ (where h is the thickness which is much smaller than any other lengthscale in the problem) are traction-free, we approximate $\sigma_{zz} = 0$ everywhere (an approximation that becomes better and better as $h \to 0$). Similarly, we have $\sigma_{zy} = \sigma_{zx} = 0$. We can therefore set $\sigma_{zz} = \sigma_{zy} = \sigma_{zx} = 0$ in Eq. (5.57) to obtain

$$
\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} \end{pmatrix} = \frac{1}{E} \begin{pmatrix} 1 & -\nu & 0 \\ -\nu & 1 & 0 \\ 0 & 0 & 1+\nu \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{pmatrix}
\tag{5.58}
$$

and

$$
\varepsilon_{zz}(x,y) = -\frac{\nu}{E}\left[\sigma_{xx}(x,y) + \sigma_{yy}(x,y)\right] .
\tag{5.59}
$$

To obtain the plane-stress analog of the Navier-Lamé Eq. (5.24) we need to invert Eq. (5.58), obtaining

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{pmatrix} = \frac{E}{1-\nu^2} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & 1-\nu \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} \end{pmatrix} , \tag{5.60}$$

which can not be simply obtained from Eq. (5.56) by removing columns and rows. We can now substitute the last relation in the 2D momentum balance equation $\nabla \cdot \boldsymbol{\sigma} = \rho \partial_{tt} \boldsymbol{u}$ (we stress again that $\boldsymbol{\sigma}$ and $\boldsymbol{u}$ are already 2D here). The resulting 2D equation reads

$$\left[\frac{\nu E}{1-\nu^2} + \frac{E}{2(1+\nu)} \right] \nabla (\nabla \cdot \boldsymbol{u}) + \left[\frac{E}{2(1+\nu)} \right] \nabla^2 \boldsymbol{u} = \rho \partial_{tt} \boldsymbol{u} , \tag{5.61}$$

which is identical in form to the Navier-Lamé Eq. (5.24) simply with a renormalized λ

$$\lambda \to \tilde{\lambda} = \frac{\nu E}{1-\nu^2} = \frac{2\nu\mu}{1-\nu} = \frac{2\lambda\mu}{\lambda+2\mu} . \tag{5.62}$$

The shear modulus μ remains unchanged

$$\tilde{\mu} = \mu = \frac{E}{2(1+\nu)} . \tag{5.63}$$

Finally, we can substitute $\sigma_{xx}(x,y)$ and $\sigma_{yy}(x,y)$ inside Eq. (5.59) to obtain $\varepsilon_{zz}(x,y)$. Note that $u_z(x,y,z) = \varepsilon_{zz}(x,y)z$ is linear in z.

Plane-strain

We now consider objects that are very thick in one dimension, say z, and are deformed in the xy-plane with no z dependence. These physical conditions are termed plane-strain and are characterized by $\epsilon_{zx} = \epsilon_{zy} = \epsilon_{zz} = 0$. Eliminating these components from Eq. (5.56) we obtain

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{pmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & 1-2\nu \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} \end{pmatrix} \tag{5.64}$$

and

$$\sigma_{zz}(x,y) = \frac{\nu E}{(1+\nu)(1-2\nu)} \left[\varepsilon_{xx}(x,y) + \varepsilon_{yy}(x,y) \right] . \tag{5.65}$$

We can now substitute Eq. (5.64) in the 2D momentum balance equation $\nabla \cdot \boldsymbol{\sigma} = \rho \partial_{tt} \boldsymbol{u}$ (where again $\boldsymbol{\sigma}$ and $\boldsymbol{u}$ are 2D). The resulting 2D equation is identical to the Navier-Lamé Eq. (5.24),

both in form and in the elastic constants. With the solution at hand, we can use Eq. (5.65) to calculate $\sigma_{zz}(x, y)$. Finally, we note that Eq. (5.64) can be inverted to

$$
\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} \end{pmatrix} = \frac{1+\nu}{E} \begin{pmatrix} 1-\nu & -\nu & 0 \\ -\nu & 1-\nu & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{pmatrix} , \tag{5.66}
$$

which can not be simply obtained from Eq. (5.57) by eliminating columns and rows. Using the last relation we can rewrite Eq. (5.65) as

$$
\sigma_{zz}(x, y) = \nu \left[\sigma_{xx}(x, y) + \sigma_{yy}(x, y) \right] . \tag{5.67}
$$

In summary, we see that in both plane-stress and plane-strain cases we can work with 2D objects instead of their 3D counterparts, which is a significant simplification. One has, though, to be careful with the elastic constants as explained above.

Airy stress function (potential)

Focus now on 2D static deformation conditions (either plane-stress or plane-strain) and write down the momentum balance equations under static conditions

$$
\partial_x \sigma_{xx} + \partial_y \sigma_{xy} = 0 \quad \text{and} \quad \partial_x \sigma_{yx} + \partial_y \sigma_{yy} = 0 . \tag{5.68}
$$

These equations are automatically satisfied if $\boldsymbol{\sigma}$ is derived from a scalar potential χ following

$$
\sigma_{xx} = \partial_{yy}\chi, \quad \sigma_{xy} = -\partial_{xy}\chi, \quad \sigma_{yy} = \partial_{xx}\chi . \tag{5.69}
$$

χ is called Airy stress potential. This implies

$$
\sigma_{xx} + \sigma_{yy} = \nabla^2 \chi . \tag{5.70}
$$

What a differential equation does χ satisfy? Obviously up to now we did not use the fact that we are talking about a linear elastic solid (we just used linear momentum balance). To incorporate the linear elastic nature of the problem we use Hooke's law, which implies

$$
\sigma_{xx} + \sigma_{yy} = \operatorname{tr} \boldsymbol{\sigma} \propto \operatorname{tr} \boldsymbol{\varepsilon} = \nabla \cdot \boldsymbol{u} . \tag{5.71}
$$

However, we already proved that $\nabla \cdot \boldsymbol{u}$ is harmonic under static conditions (cf. Eq. (5.33)), leading to $\nabla^2(\sigma_{xx} + \sigma_{yy}) = 0$, which in turn implies

$$
\nabla^2 \nabla^2 \chi = 0 . \tag{5.72}
$$

Therefore, χ satisfies the bi-Laplace equation, i.e. it is a bi-harmonic function.

Example: Cylindrical cavity

Consider a large linear elastic solid containing a cylindrical hole of radius R under uniform radial tensile loading σ^∞ far away (plane-strain conditions). The hole can be regarded as a defect inside a perfect solid. What is the emerging stress field? What can we learn from it? First, the geometry of the problem suggests we should work in polar coordinates (derive)

$$\left(\partial_{rr} + \frac{\partial_r}{r} + \frac{\partial_{\theta\theta}}{r^2}\right)\left(\partial_{rr} + \frac{\partial_r}{r} + \frac{\partial_{\theta\theta}}{r^2}\right)\chi(r,\theta) = 0 \tag{5.73}$$

and

$$\sigma_{rr} = \frac{\partial_r\chi}{r} + \frac{\partial_{\theta\theta}\chi}{r^2}, \quad \sigma_{r\theta} = -\partial_r\left(\frac{\partial_\theta\chi}{r}\right), \quad \sigma_{\theta\theta} = \partial_{rr}\chi . \tag{5.74}$$

Furthermore, azimuthal symmetry implies $\sigma_{r\theta} = 0$ and no θ-dependence. Moreover, since the only lengthscale in the problem is R, we expect the result to be a function of r/R alone. Finally, linearity implies that σ_{rr} and $\sigma_{\theta\theta}$ are proportional to σ^∞. We should now look for θ-independent solutions of the bi-harmonic equation of (5.72) with the following boundary conditions

$$\sigma_{rr}(r=R) = 0 \quad \text{and} \quad \sigma_{rr}(r\to\infty) = \sigma^\infty . \tag{5.75}$$

The θ-independent solutions of Eq. (5.73) are r^2, $\log r$ and $r^2 \log r$ (show that $\chi(r,\theta) = \phi_0(r,\theta) + \phi_1(r,\theta)r\cos\theta + \phi_2(r,\theta)r\sin\theta + \phi_3(r,\theta)r^2$ is the general solution of the bi-harmonic equation, where $\{\phi_i(r,\theta)\}$ are harmonic). The $r^2 \log r$ solution gives rise to a logarithmically diverging stress as $r\to\infty$, and hence should be excluded here. We therefore have

$$\chi(r) = a\log r + br^2 . \tag{5.76}$$

Satisfying the boundary conditions implies that $a = -\sigma^\infty R^2$ and $b = \sigma^\infty/2$, leading to

$$\sigma_{rr} = \sigma^\infty\left(1 - \frac{R^2}{r^2}\right), \quad \sigma_{\theta\theta} = \sigma^\infty\left(1 + \frac{R^2}{r^2}\right) . \tag{5.77}$$

Note that $\sigma_{\theta\theta}$ at the surface of the cylinder, which tends to break the material apart, is two times larger than σ^∞. This (mild) amplification factor is a generic property of defects which plays a crucial role in determining the strength of solids. We will discuss this later in the course when dealing with failure. Another interesting feature of the solution is that $\sigma_{\theta\theta} + \sigma_{rr}$ is a constant.

Complex variable methods are applicable to Eq. (5.72) as well. We first rewrite it in terms of complex differential operators as

$$\partial_{zz}\partial_{\bar{z}\bar{z}}\chi = 0 \ . \tag{5.78}$$

It is obvious that analytic functions are solutions of this equation. However, there are more solutions because of the appearance of another derivative with respect to $\bar{z}$. In fact it is clear that $\bar{z}f(z)$, where $f(z)$ is an analytic function, is also a solution. As no other solutions can be found, the most general solution of the bi-Laplace equation is given in terms of *two* analytic functions $f(z)$ and $g(z)$ as

$$\chi = \Re\left[\bar{z}f(z) + g(z)\right] \ . \tag{5.79}$$

Of course the imaginary part can be used as well. It is important to understand that while this solution is given in terms of analytic function it is by itself not an analytic function. The reason is obvious: it depends on $\bar{z}$. The stress tensor can be easily derived using complex derivatives, yielding (derive)

$$\sigma_{xx} + \sigma_{yy} = 4\Re\left[f'(z)\right] \ , \tag{5.80}$$

$$\sigma_{yy} - \sigma_{xx} + 2i\sigma_{xy} = 2\left[\bar{z}f''(z) + g''(z)\right] \ . \tag{5.81}$$

Finally, we note that while the bi-Laplace equation is *not* conformally invariant (prove), conformal methods are useful for its solution.

C. Elastic waves

Up to now we did not discuss dynamic phenomena. However, the most basic solutions of the Navier-Lamé Eq. (5.24) are dynamic and well-known to you from everyday life: elastic waves. This might appear strange at first sight because the Navier-Lamé Eq. (5.24) does not take the form of an ordinary wave equation. The reason will become clear soon. The first step to address this question would be to decompose the general displacement field $\boldsymbol{u}$ into a curl-free component and a divergence-free component (Helmholtz decomposition)

$$\boldsymbol{u} = \nabla\phi + \nabla \times \boldsymbol{\psi} \ , \tag{5.82}$$

where ϕ and $\boldsymbol{\psi}$ are scalar and vector displacement potentials, respectively. Recall that $\nabla\cdot(\nabla\times\boldsymbol{\psi}) = 0$ and $\nabla \times (\nabla\phi) = 0$. Note that the vector potential features a gauge freedom, i.e. $\boldsymbol{\psi} \to \boldsymbol{\psi} + \nabla\varphi$ with a scalar field φ leaves $\boldsymbol{u}$ unchanged. A common gauge choice is $\nabla \cdot \boldsymbol{\psi} = 0$ (e.g. as adopted in seismology). In 2D, it can be satisfied by choosing $\boldsymbol{\psi} = \psi_z(x,y,t)\,\hat{z}$.

Substituting Eq. (5.82) into the Navier-Lamé Eq. (5.24), we obtain

$$\nabla \left[(\lambda + 2\mu)\nabla^2 \phi - \rho \partial_{tt} \phi \right] + \nabla \times \left[\mu \nabla^2 \boldsymbol{\psi} - \rho \partial_{tt} \boldsymbol{\psi} \right] = 0 \ . \tag{5.83}$$

Using the analogy of this equation with Eq. (5.82) we see that each term in the square bracket should vanish independently, yielding

$$c_d^2 \nabla^2 \phi = \partial_{tt} \phi \quad \text{and} \quad c_s^2 \nabla^2 \boldsymbol{\psi} = \partial_{tt} \boldsymbol{\psi} \ , \tag{5.84}$$

where

$$c_d = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad c_s = \sqrt{\frac{\mu}{\rho}} \ , \tag{5.85}$$

are the dilatational (longitudinal, sound) and shear wave speeds, respectively. Linear elastodynamics is therefore characterized by two different wave equations with two different wave speeds, $c_d > c_s$ (recall that $\lambda > -2\mu/3$, which implies $\lambda + 2\mu > 4\mu/3 > \mu$). In that sense, while this theory shares various features with electrodynamics (electromagnetism), it is more complicated because of the presence of two wave speeds instead of one (the speed of light). It is also important to note that while the two wave equations in (5.84) are independent inside the bulk of the solid, they are coupled on the boundaries, which of course makes things more complicated (we will see this explicitly when discussing fracture later in the course). Finally, note that there exist also surface (Rayleigh) waves whose propagation velocity c_R is different from both c_s and c_d. In general, we have $c_R < c_s < c_d$.

How do we actually know that c_s corresponds to shear waves and c_d to dilatational waves? This is implicit in the fact that the latter are curl-free and the former are divergence-free, but can we find more explicit distinguishing features? To that aim, consider plane-wave solutions of the form

$$\boldsymbol{u} = g(\boldsymbol{x} \cdot \boldsymbol{n} - c\,t)\boldsymbol{a} \ , \tag{5.86}$$

where $\boldsymbol{n}$ is the propagation direction, $\boldsymbol{a}$ is the direction of the displacement and $|\boldsymbol{n}| = |\boldsymbol{a}| = 1$. Substituting this expression into the Navier-Lamé Eq. (5.24), we obtain (see tutorial)

$$(c_d^2 - c_s^2)(\boldsymbol{a} \cdot \boldsymbol{n})\boldsymbol{n} + (c_s^2 - c^2)\boldsymbol{a} = 0 \ . \tag{5.87}$$

There are two independent solutions to this equation; either $c = c_s$ and $\boldsymbol{a} \cdot \boldsymbol{n} = 0$ <u>or</u> $c = c_d$ and $\boldsymbol{a} \cdot \boldsymbol{n} = \pm 1$ (recall that both $\boldsymbol{n}$ and $\boldsymbol{a}$ are unit vectors). Therefore, shear waves are polarized such that the displacement is always orthogonal to the propagation direction and dilatational waves

are polarized such that the displacement is parallel to the propagation direction.

Dilatational (pressure/density) waves in fluids and solids

Let us briefly discuss the difference between dilatational (pressure/density) waves in fluids and solids. Since we consider linear waves we can neglect convective nonlinearities and hence the momentum balance equation for both fluids and solids reads

$$\rho \partial_t \boldsymbol{v} = \nabla \cdot \boldsymbol{\sigma} \ . \tag{5.88}$$

The difference stems from the different constitutive laws that relate the stress tensor $\boldsymbol{\sigma}$ to particles motions. To see this, we use Eq. (5.19) to write Hooke's law as

$$\boldsymbol{\sigma} = K \operatorname{tr} \boldsymbol{\varepsilon} \boldsymbol{I} + 2\mu \left(\boldsymbol{\varepsilon} - \frac{1}{3} \operatorname{tr} \boldsymbol{\varepsilon} \boldsymbol{I} \right) \ . \tag{5.89}$$

For a fluid we have $\mu = 0$, i.e. fluids cannot sustain shear stresses at all (note that since we focus on non-dissipative waves we exclude viscous stresses here). Consider then small density perturbations, $\rho = \rho_0 + \delta\rho$, such that

$$\operatorname{tr} \boldsymbol{\varepsilon} = \frac{\delta V}{V} = -\frac{\delta\rho}{\rho_0} \ . \tag{5.90}$$

Therefore, to linear order in density perturbations the momentum balance equation for fluids reads

$$\rho_0 \partial_t \boldsymbol{v} = -\frac{K}{\rho_0} \nabla \rho \ . \tag{5.91}$$

Operating with the divergence operator on both sides of this equation we obtain

$$\rho_0 \partial_t \nabla \cdot \boldsymbol{v} = -\frac{K}{\rho_0} \nabla^2 \rho \ . \tag{5.92}$$

Finally, linearizing the mass conservation equation of (4.5)

$$\partial_t \rho + \rho_0 \nabla \cdot \boldsymbol{v} = 0 \ , \tag{5.93}$$

we obtain

$$\partial_{tt} \rho = \frac{K}{\rho_0} \nabla^2 \rho \ . \tag{5.94}$$

Therefore, the speed of sound (dilatational/desnity/pressure waves) in fluids is $\sqrt{K/\rho_0}$. What happens in solids? One may naively think that even though solids feature a finite shear modulus μ,

the combination $\boldsymbol{\varepsilon} - \frac{1}{3}\operatorname{tr}\boldsymbol{\varepsilon}\,\boldsymbol{I}$ — which describes shear/deviatoric deformation — does not contribute to dilatational waves. This is wrong. In fact, we have

$$\nabla \cdot \left(\boldsymbol{\varepsilon} - \frac{1}{3}\operatorname{tr}\boldsymbol{\varepsilon}\,\boldsymbol{I} \right) = \frac{2}{3}\nabla \operatorname{tr}\boldsymbol{\varepsilon} - \frac{1}{2}\nabla \times (\nabla \times \boldsymbol{u}) \ . \tag{5.95}$$

That is, $\boldsymbol{\varepsilon}^{dev} = \boldsymbol{\varepsilon} - \frac{1}{3}\operatorname{tr}\boldsymbol{\varepsilon}\,\boldsymbol{I}$ is trace-less, but not divergence-free. Using this result in the momentum balance equation (through Hooke's law) and operating with the divergence operator on both sides we obtain

$$\rho_0 \partial_t \nabla \cdot \boldsymbol{v} = \left(K + \frac{4\mu}{3} \right) \nabla^2 \operatorname{tr}\boldsymbol{\varepsilon} \ . \tag{5.96}$$

Following the steps as in the fluid case, we immediately see that the speed of sound in solids is $\sqrt{\frac{K + \frac{4\mu}{3}}{\rho_0}}$, which is of course identical to the result obtained in Eq. (5.85) since $K + \frac{4\mu}{3} = \lambda + 2\mu$. We thus conclude that the shear modulus contributes to the speed of sound in solids, which is different from the speed of sound in fluids.

VI.   THE LINEARIZED FIELD THEORY OF THERMO-ELASTICITY

What happens when additional fields play a role? Up to now we did not consider explicitly the role of temperature. We know that ordinary solids expand when heated. Therefore, we expect that differential heating, i.e. temperature gradients, would give rise to nontrivial thermal stresses. Such processes are important in a wide range of physical systems, from heat engines, through blood vessels to the deformation of the earth. In situations in which the temperature T plays a role, the relevant thermodynamic potential is the Helmholtz free energy, which is obtained by a Legendre transformation of the internal energy

$$f(\boldsymbol{\varepsilon}, T) = u(\boldsymbol{\varepsilon}, T) - T\, s(\boldsymbol{\varepsilon}, T) \ . \tag{6.1}$$

Therefore, the second law of thermodynamics (dissipation inequality) in Eq. (4.38) reads

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{f} - s\dot{T} \geq 0 \ , \tag{6.2}$$

where we identified $\boldsymbol{D} = \dot{\boldsymbol{\varepsilon}}$. Using the chain rule to express $\dot{f}$, we obtain

$$\left(\boldsymbol{\sigma} - \frac{\partial f}{\partial \boldsymbol{\varepsilon}} \right) : \dot{\boldsymbol{\varepsilon}} - \left(s + \frac{\partial f}{\partial T} \right) \dot{T} \geq 0 \ . \tag{6.3}$$

Since elastic response in reversible, we expect an equality to hold. Moreover, the strain and the temperature can be varied independently. Therefore, the second law analysis implies

$$\boldsymbol{\sigma} = \frac{\partial f}{\partial \boldsymbol{\varepsilon}} \quad \text{and} \quad s = -\frac{\partial f}{\partial T} \ . \tag{6.4}$$

These relations are the macro-canonical counterparts of Eqs. (5.4). What form then $f(\boldsymbol{\varepsilon}, T)$ can take within a linear theory? Obviously the temperature independent terms in Eq. (5.11) still appear. To couple temperature variations to deformation we need to construct a scalar, which within a linear theory must take the form $(T - T_0)\, \mathrm{tr}\, \boldsymbol{\varepsilon}$ (where T_0 is some reference temperature). Therefore, $f(\boldsymbol{\varepsilon}, T)$ takes the form

$$f(\boldsymbol{\varepsilon}, T) = \frac{1}{2} K (\mathrm{tr}\, \boldsymbol{\varepsilon})^2 + \mu \left(\varepsilon_{ij} - \frac{1}{3} \mathrm{tr}\, \boldsymbol{\varepsilon} \delta_{ij} \right)^2 - K \alpha_T \, (T - T_0)\, \mathrm{tr}\, \boldsymbol{\varepsilon} + f_0(T) \ , \tag{6.5}$$

where the physical meaning of α_T will become clear soon and $f_0(T)$ is a temperature dependent function that plays no role here. The constitutive relation reads

$$\sigma_{ij} = -K \alpha_T \, (T - T_0)\, \delta_{ij} + K\, \mathrm{tr}\, \boldsymbol{\varepsilon} \delta_{ij} + 2\mu (\varepsilon_{ij} - \frac{1}{3} \mathrm{tr}\, \boldsymbol{\varepsilon} \delta_{ij}) \ . \tag{6.6}$$

First consider free thermal expansion of a body (i.e. the temperature is increased from T_0 to T). In this case no stresses emerge, $\boldsymbol{\sigma} = 0$ (why is this the case?), and the deformation is isotropic, hence Eq. (6.6) implies

$$\text{tr}\,\boldsymbol{\varepsilon} = \alpha_T\,(T - T_0)\ .\tag{6.7}$$

Since $\text{tr}\,\boldsymbol{\varepsilon}$ is the relative volume change, $\delta V/V$, α_T is simply the thermal expansion coefficient $\alpha_T = \frac{1}{V}\frac{\partial V}{\partial T}$.

A side comment: While the thermal expansion coefficient appears as a linear response coefficient, it is not a harmonic (linear) material property (i.e. it cannot be obtained from a quadratic approximation to the energy). To see this, convince yourself that the thermal average $\delta V = V <\text{tr}\,\boldsymbol{\varepsilon}>_T$ vanishes when a quadratic approximation to the energy, $u \sim (\text{tr}\,\boldsymbol{\varepsilon})^2$, is used. You need to go nonlinear, i.e. invoke anharmonic contributions to the energy.

The equations of motion for a linear thermo-elastic solid take the form (neglecting inertia and body forces, and using λ and μ again)

$$(\lambda + \mu)\nabla\,(\nabla \cdot \boldsymbol{u}) + \mu\nabla^2\boldsymbol{u} = \alpha_T\,K\nabla T\ .\tag{6.8}$$

This shows that thermal gradients appear as a source term (inhomogeneous term) in the standard linear elastic equations of motion.

Example: Heated annulus

Consider a thin annulus of internal radius R_1 and external radius R_2. Consider then a nonuniform, purely radial, temperature field $T(r)$ and determine the resulting displacement field. The geometry of the problem implies that the only non-vanishing displacement component is $u_r(r,\theta) = u(r)$. Writing then Eqs. (6.8) in polar coordinates we obtain

$$\partial_{rr}u + \frac{\partial_r u}{r} - \frac{u}{r^2} = \frac{\alpha_T\,K}{\lambda + 2\mu}\partial_r T\ .\tag{6.9}$$

What are the boundary conditions? As the inner and outer surfaces of the annulus are traction-free, we have the following boundary conditions

$$\sigma_{rr}(r = R_1) = \sigma_{rr}(r = R_2) = 0\ .\tag{6.10}$$

The key point for solving Eq. (6.9) is to note that the operator on the left-hand-side can be rewritten in compact form as

$$\partial_{rr}u + \frac{\partial_r u}{r} - \frac{u}{r^2} = \partial_r\left[\frac{\partial_r(r\,u)}{r}\right]\ .\tag{6.11}$$

Therefore, integrating twice Eq. (6.9) readily yields

$$u(r) = \frac{\alpha_T \, K}{\lambda + 2\mu} \frac{1}{r} \int_{R_1}^{r} T(r')r'dr' + \frac{c_1 r}{2} + \frac{c_2}{r} \ , \tag{6.12}$$

where c_1 and c_2 are two integration constants. These are being determined (derive) by the traction-free boundary conditions of Eq. (6.10) and turn out to be proportional to $\int_{R_1}^{R_2} T(r')r'dr'$. Are these results valid for $T(r) = $ const., i.e. for a spatially uniform temperature field?

VII.   THE NON-LINEAR FIELD THEORY ELASTICITY

Our previous discussion focussed on linear elastic deformation. Why is it such a useful theory? After all it is a linear perturbation theory, so what makes it so relevant in a wide range of situations? In other words, why ordinary solids do not typically experience large elastic deformations? The answer is hidden in a small parameter that we have not yet discussed. Until now the only material parameter of stress dimensions was the elastic modulus, say μ. In ordinary solids the elastic modulus is large. Compared to what? What other typical, intrinsic, stress scales exist? The answer is that ordinary solids start to respond irreversibly (flow plastically, break, etc.) at a typical stress level that is usually much smaller than the elastic modulus. In other words, reversibility breaks down at a typically small displacement gradient. As reaching the onset of irreversibility limit still requires relatively large stresses, this explains why a small elastic deformation perturbation theory is useful. We will focuss on irreversible processes later in the course.

Everyday life experience, however, tells us that there are many materials that respond reversibly at large deformation. Think, for example, of a rubber band, of your skin or of jelly. Such materials can deform to very large strains (of order unity or more) under mild stresses and recover their original shape when the stress is removed. They are "soft". Such soft materials are of enormous importance and range of applicability, and have attracted lots of attention in recent years. What makes them significantly softer than ordinary solids? The answer is that their elasticity has a difference origin.

A.   Entropic elasticity ("Rubber elasticity")

The paradigmatic example of an elastic behavior is a Hookean spring in which a restoring force is exerted in response to length/shape variations. In this case, the restoring force has an energetic origin: the interatomic interaction energy changes with the length/shape variations. However, this is not the only form of an elastic behavior. Consider the Helmholtz free energy density

$$f(\boldsymbol{E}, T) = u(\boldsymbol{E}, T) - T\, s(\boldsymbol{E}, T) \ , \tag{7.1}$$

where $\boldsymbol{E}$ now is the Green-Lagrange (metric) strain tensor. A stress measure is obtained by the variation of f with respect to $\boldsymbol{E}$. Ordinary elasticity of "hard" materials, e.g. of metals, has an energetic origin. In this case the entropy s does not depend on the deformation, while the internal

energy u does. On the other hand, "rubber" elasticity of "soft" materials, e.g. of gels, rubber and various polymeric materials, has an entropic origin. In this case, the internal energy does not depend on the deformation, but the entropy does.

To understand the physics underlying entropic elasticity we consider a network of long-chain polymers within a fixed unit volume. We assume that the network is incompressible. Consider first a single polymer chain of length $L = m\ell$, where m is the number of monomers and ℓ is the length of a single monomer. Suppose now that one end of the chain is fixed (say at the origin) and the other end is free to wander in space. Denote the end-to-end vector by $\boldsymbol{r}$. In situations in which $r = |\boldsymbol{r}| \ll L$ and under the assumption that there is no correlation between the orientation of successive monomers, the probability distribution function of the end-to-end distance $p(r)$ can be easily determined, in analogy to a random walk in time, to be

$$p(r) \propto e^{-\frac{3r^2}{2\langle r^2 \rangle}} \,, \tag{7.2}$$

where $\langle r^2 \rangle = m\,\ell^2$ is the mean-square value of r (in the analogy to random walk in time, m plays the role of time t). $p(r)$ measures the number of *configurations* the chain can be in for a given end-to-end distance r. Also note that no elastic energy is involved here, i.e. the "joints" of size ℓ can move freely (in principle, ℓ can be larger than the monomer size, i.e. the so-called persistence length above which correlations fade away. In this case, the polymer is termed "semi-flexible", but we do not discuss this here). A chain with these properties is termed a Gaussian chain (note that despite the name, $p(r)$ of Eq. (7.2) is not strictly Gaussian, but rather takes the form $p(r) = 4\pi r^2 \left(\frac{3}{2\,\pi\langle r^2\rangle}\right)^{3/2} e^{-\frac{3r^2}{2\langle r^2\rangle}}$, featuring $p(0) = 0$ and $r > 0$. Consequently, one can say that $p(r)$ is predominantly Gaussian). The configurational entropy of a single polymer chain with an end-to-end distance r is given by

$$\bar{s} = s_0 + k_B \ln\left[p(r)\right] = \bar{s}_0 - k_B \frac{3r^2}{2\langle r^2\rangle} \,, \tag{7.3}$$

where s_0 and $\bar{s}_0$ are unimportant constants. In order to understand the effect of deformation on the entropy of the ith polymer chain we denote the undeformed end-to-end distance by $\boldsymbol{r}^{(i)} = (X_1^{(i)}, X_2^{(i)}, X_3^{(i)})$ and the deformed one by $\tilde{\boldsymbol{r}}^{(i)} = (x_1^{(i)}, x_2^{(i)}, x_3^{(i)}) = (\lambda_1^{(i)} X_1^{(i)}, \lambda_2^{(i)} X_2^{(i)}, \lambda_3^{(i)} X_3^{(i)})$, where $\{\lambda_{k=1-3}^{(i)}\}$ are the (principal) stretches. Therefore, the entropy change of a single chain due to deformation reads

$$\Delta \bar{s}^{(i)} = -\frac{3k_B}{2\langle r^2\rangle} \left(([\lambda_1^{(i)}]^2 - 1)[X_1^{(i)}]^2 + ([\lambda_2^{(i)}]^2 - 1)[X_2^{(i)}]^2 + ([\lambda_3^{(i)}]^2 - 1)[X_3^{(i)}]^2\right) \,. \tag{7.4}$$

We now assume that the deformation is *affine*, i.e. that the macroscopic and microscopic strains are the same, $\lambda_k^{(i)} = \lambda_k$. Hence, the entropy change per unit volume of the part of the polymeric network that contains N chains and occupies a volume V reads

$$s = \sum_{i=1}^{N} \frac{\Delta \bar{s}^{(i)}}{V} = \tag{7.5}$$

$$-\frac{3k_B}{2V\langle r^2 \rangle}\left((\lambda_1^2 - 1)\sum_{i=1}^{N}[X_1^{(i)}]^2 + (\lambda_2^2 - 1)\sum_{i=1}^{N}[X_2^{(i)}]^2 + (\lambda_3^2 - 1)\sum_{i=1}^{N}[X_3^{(i)}]^2 \right) \ .$$

We now invoke isotropy and assume that we can treat $\{[X_k^{(i)}]^2\}$ as independent variables, to obtain

$$\sum_{i=1}^{N}[X_1^{(i)}]^2 = \sum_{i=1}^{N}[X_2^{(i)}]^2 = \sum_{i=1}^{N}[X_3^{(i)}]^2 = \frac{1}{3}N\langle r^2 \rangle \ . \tag{7.6}$$

Therefore, the free energy density of the polymeric network (due to deformation) is given by

$$f = -Ts = \frac{1}{2}nk_BT\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3 \right) \ , \tag{7.7}$$

where $n \equiv N/V$ is the number of chains per unit volume (density of chains). Recall that we also assume incompressibility (consequently we did not consider the variation of the entropy with volume changes), i.e. that the constitutive law also includes the incompressibility condition

$$J = \det \boldsymbol{F} = \lambda_1\lambda_2\lambda_3 = 1 \ . \tag{7.8}$$

We can immediately identify nk_BT in Eq. (7.7) as an elastic modulus (it has the dimensions of energy density, i.e. of stress), which actually corresponds to the shear modulus

$$\mu = nk_BT \ . \tag{7.9}$$

This dependence on T, i.e. $d\mu/dT > 0$, has remarkable consequences that distinguish entropic elasticity from energetic one. For example, a piece of rubber under a fixed force will shrink/expand in response to heating/cooling, just the opposite of the behavior of a metallic spring! Another related effect, that we do not discuss in detail here, is that of adiabatic stretching. When we rapidly (and elastically) stretch a piece of metal it cools down. However, a rubber band under the same conditions warms up. You can easily experience it yourself by rapidly stretching a piece of rubber and using your lips as a thermo-sensitive device. We note that f, which was calculated above, is the free-energy in the deformed configuration per unit volume in the undeformed configuration.

Equations (7.7)-(7.8) constitute the incompressible neo-Hookean model, which is one of the first and most useful nonlinear elastic models. The statistical mechanical model that was used to

derived it, originally due to Flory in the early 1940's, is called the Gaussian-chain model. The name "neo-Hookean" has to do with the intimate relation of this model to the small strains linear elastic Hookean model. Noting that

$$\text{tr}\, \boldsymbol{E} = \frac{1}{2}\text{tr}(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}) = \frac{1}{2}\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3\right) \ , \tag{7.10}$$

we can rewrite Eq. (7.7) as

$$f = \mu\, \text{tr}\, \boldsymbol{E} = \frac{1}{2}\mu\left[\text{tr}(\boldsymbol{F}^T\boldsymbol{F}) - 3\right] \ . \tag{7.11}$$

We can incorporate Eq. (7.8) into this free-energy function by writing

$$f = \frac{1}{2}\mu\left[\text{tr}(\boldsymbol{F}^T\boldsymbol{F}) - 3\right] - \alpha\left(J - 1\right) \ , \tag{7.12}$$

where α is a Lagrange multiplier introduced to enforce incompressibility. This is the simplest possible model that is quadratic in $\boldsymbol{F}$ and reduces to Hookean elasticity at small stretches. This phenomenological approach cannot, of course, predict the exact expression of μ in Eq. (7.9), which requires a statistical mechanical derivation, though the T-dependence is expected on general grounds. Note also that unlike Hookean linear elasticity the neo-Hookean model is rotationally invariant under **finite** rotations and is also objective.

We note in passing that we can allow for volume variations (i.e. give up the incompressibility constraint), in which case the Gaussian-chain model would yield

$$f = \frac{1}{2}\mu\left[\text{tr}(\boldsymbol{F}^T\boldsymbol{F}) - 3 - 2\log J\right] \ , \tag{7.13}$$

which simply accounts for the entropic contribution due to volume variations (note that an increase in volume, i.e. in J, results in an increase of entropy/number of available configurations, hence in a reduction in f). More elaborated models of compressible neo-Hookean-like materials include additional functions of $J - 1$ in the free-energy.

To appreciate the "softness" of materials that are governed by entropic (rubber-like) elasticity, let us make some rough estimates. First consider ordinary (say, metallic) solids. The elastic modulus has the dimensions of stress, which is equivalent to energy density. The typical energy scale for metals is roughly 1eV. Divide this by an atomic volume, $\Omega \simeq 10^{-29}\text{m}^3$, and you get 10GPa which is a reasonable rough estimate (the Young's modulus of metals can reach 100GPa). Consider now Eq. (7.9), $\mu = nk_BT$. At room temperature we have $k_BT_\text{R} \simeq 1/40 eV$, which sets the energy scale for rubber elasticity. If we assume a chain density n of 10^{-2} per atomic volume, we get an elastic modulus which is about 3 orders of magnitude smaller for rubber. Indeed,

10MPa is a reasonable rough estimate for the modulus of rubber. When we consider gels, which are typically filled with water (or other solvents), the effective chain density can be significantly smaller and the modulus drops down to the 10KPa range, which is 6 orders of magnitude smaller than ordinary solids. These rigidity levels are also characteristic of biological substance such as tissues and cells.

B. Geometric nonlinearities and stress measures

Many other useful nonlinear elastic models were developed based on either statistical mechanical or phenomenological approaches that employ symmetry principles and experimental observations. It is usually very difficult to solve nonlinear elastic problems analytically. The inherent difficulty goes beyond the usual statement that nonlinear differential equations are not analytically tractable in general. The reason for that is geometrical in nature and has to do with the fact that in nonlinear elastic problems the domain in which we solve the differential equations depends itself on the solution that is sought for (and of course unknown to begin with). Think, for example, of the Cauchy stress $\boldsymbol{\sigma}$, defined as the force per unit area in the deformed configuration, and consider a free boundary. Since the boundary is traction-free, $\sigma_{nn} = \sigma_{tn} = 0$ on it, where n and t denote the normal and tangent to the free boundary, respectively. In order to satisfy this boundary condition throughout the deformation process, the location should be known, but this usually requires to know the solution. We did not encounter this problem in the linearized theory since the deformed and undeformed are distinguishable only to second order in the displacement gradient.

One way to deal with this situation is to formulate problems in the undeformed configuration. This was briefly discussed in Eqs. (3.37), (3.38) and (4.20), and will be repeated here within a thermodynamic context. Consider a small incremental deformation of a body (that might be already deformed) and ask how much stress work was done within a volume element $\delta \boldsymbol{x}^3$. For that aim, define an incremental strain measure $d\epsilon$ as the change in length of a material element relative to the current (deformed) state of the material. To stress the difference between ϵ and ε, we resort to 1D and we discuss again Eqs. (3.19)-(3.20). ε is defined as the change in length with respect to the undeformed state ℓ_0, $\ell - \ell_0$, relative to the undeformed state

$$d\varepsilon = \frac{d\ell}{\ell_0} \quad \Longrightarrow \quad \varepsilon = \int_{\ell_0}^{\ell} \frac{d\ell}{\ell_0} = \frac{\ell - \ell_0}{\ell_0} = \lambda - 1 \quad \Longrightarrow \quad \lambda = \varepsilon + 1 \ , \tag{7.14}$$

where $\lambda = \ell/\ell_0$ is the stretch. $d\epsilon$ is defined similarly to $d\varepsilon$, but with respect to the deformed

(current) state, implying

$$d\epsilon = \frac{d\ell}{\ell} \quad \Longrightarrow \quad \epsilon = \int_{\ell_0}^{\ell} \frac{d\ell}{\ell} = \ln\left(\frac{\ell}{\ell_0}\right) = \ln\lambda \quad \Longrightarrow \quad \lambda = e^{\epsilon} . \tag{7.15}$$

While these two strain measures (as every other two strain measures) agree to linear order, they differ dramatically in general; $\lambda(\varepsilon)$ is a linear function, while $\lambda(\epsilon)$ is exponential. Going back to our original question, the stress work done by the Cauchy stress $\boldsymbol{\sigma}$ in the (current) volume element $\delta\boldsymbol{x}^3$ is

$$\boldsymbol{\sigma} : d\boldsymbol{\epsilon}\, \delta\boldsymbol{x}^3 , \tag{7.16}$$

where $d\boldsymbol{\epsilon}$ is a tensorial generalization of $d\epsilon$ (cf. Eq. (3.23), where a slightly different notation was used). We can now associate a new stress measure that is thermodynamically conjugate to a given strain measure by demanding that the stress work produced would equal the above expression. To see how this works let us focus on the case in which the deformation measure we use is $\boldsymbol{F}$, which connects the deformed (reference) and undeformed (current) configurations. Since $\boldsymbol{F}$ is defined in terms of the reference coordinates $\boldsymbol{X}$, the relevant volume element is $\delta\boldsymbol{X}^3$. We then define a stress tensor $\boldsymbol{P}$ such that

$$\boldsymbol{P} : d\boldsymbol{F}\, \delta\boldsymbol{X}^3 = \boldsymbol{\sigma} : d\boldsymbol{\epsilon}\, \delta\boldsymbol{x}^3 . \tag{7.17}$$

$\boldsymbol{P}$ is the first Piola-Kirchhoff stress tensor, that was already defined in Eq. (3.37) using other considerations, which is related to $\boldsymbol{\sigma}$ through Eq. (3.38), $\boldsymbol{P} = J\boldsymbol{\sigma}\boldsymbol{F}^{-T}$. This is perfectly consistent (prove) with the thermodynamic definition of Eq. (7.17). It is very important to note that $\boldsymbol{P} : d\boldsymbol{F}$ is a work increment in the deformed (current) configuration per unit volume in the reference configuration. Since df has the very same meaning, we can identify $df = \boldsymbol{P} : d\boldsymbol{F}$ which leads to

$$\boldsymbol{P} = \frac{\partial f}{\partial \boldsymbol{F}} . \tag{7.18}$$

Therefore, $\boldsymbol{P}$ is the force per unit area in the reference configuration acting on its image in the deformed (current) configuration. These quantities might appear (very?) strange at first sight (even at the second and third ones), but they are enormously useful in real calculations since these can be done in the reference configuration. For that aim, we need to express the momentum balance equation in terms of $\boldsymbol{P}$ in the reference configuration, which was already done in Eq. (4.20).

As we said above, this procedure can be followed for *any* strain measure. As another example, consider the Green-Lagrange strain tensor $\boldsymbol{E}$. In that case we define a stress measure $\boldsymbol{S}$, termed the second Piola-Kirchhoff stress tensor, such that $df = \boldsymbol{S} : d\boldsymbol{E}$. Therefore,

$$\boldsymbol{S} = \frac{\partial f}{\partial \boldsymbol{E}} . \tag{7.19}$$

This stress measure is rather commonly used.

To demonstrate how these stress measures (and the associated geometric nonlinearities) appear in physical situations, let us consider the incompressible neo-Hookean material characterized by

$$f = \frac{\mu}{2} \left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - 3 \right) \tag{7.20}$$

and

$$\det \boldsymbol{F} = \lambda_1 \lambda_2 \lambda_3 = 1 \ , \tag{7.21}$$

where λ_i are the principal stretches. Consider a cylinder under a uniaxial stress state with $P_1 = P > 0$ (along the main axis of the cylinder) and $P_2 = P_3 = 0$ (traction-free lateral boundaries). The stretches take the form $\lambda_1 = \lambda$ and $\lambda_2 = \lambda_3 = \lambda^{-1/2}$, where we used isotropy and incompressibility. The relation between the Cauchy stress and the first Piola-Kirchhoff stress reads (recall that $J = \det \boldsymbol{F} = 1$)

$$\sigma = \lambda P \ . \tag{7.22}$$

Eq. (7.18) implies that in our uniaxial example we simply have $P = \partial f / \partial \lambda$ (this is proved below). Therefore, we have

$$f = \frac{\mu}{2} \left(\lambda^2 + 2\lambda^{-1} - 3 \right) \quad \Longrightarrow \quad P = \frac{\partial f}{\partial \lambda} = \mu \left(\lambda - \lambda^{-2} \right) \ . \tag{7.23}$$

The constitutive relation $P = \mu \left(\lambda - \lambda^{-2} \right)$ is different from the constitutive relation

$$\sigma = \lambda P = \mu \left(\lambda^2 - \lambda^{-1} \right) \tag{7.24}$$

due to deformation-induced nonlinearities. Note that all of these effects disappear when we linearize with respect to ε ($\lambda = 1 + \varepsilon$)

$$\sigma \simeq P \simeq 3\,\mu\,\varepsilon = E\,\varepsilon \ . \tag{7.25}$$

Therefore, $E = 3\mu$ is the Young's modulus (did you expect this? what is Poisson's ratio of this material?). One immediate consequence of nonlinearities in the constitutive law is that the symmetry between tension and compression observed in the linear theory is typically broken. We will now work out a few examples to demonstrate the rather dramatic physical effects that emerge in nonlinear elasticity.

In the example above, it was stated/argued that $P = \partial f / \partial \lambda$ is satisfied along the uniaxial tension axis. Let us prove it. Our starting point is the free-energy functional in Eq. (7.12), where

α is a Lagrange multiplier introduced to enforce incompressibility (i.e. $\partial f/\partial\alpha=0$ implies $J=1$). Recalling that $\partial\,\mathrm{tr}(\boldsymbol{F}^T\boldsymbol{F})/\partial\boldsymbol{F}=2\boldsymbol{F}$ and $\partial\det\boldsymbol{F}/\partial\boldsymbol{F}=\det\boldsymbol{F}\,\boldsymbol{F}^{-T}$, we obtain

$$\boldsymbol{P} = \frac{\partial f}{\partial\boldsymbol{F}} = \mu\boldsymbol{F} - \alpha\,\det\boldsymbol{F}\boldsymbol{F}^{-T}\ . \tag{7.26}$$

Consider then, as above, a deformation state of the form

$$\boldsymbol{F} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}\ , \tag{7.27}$$

which implies

$$\boldsymbol{P} = \mu\begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} - \alpha\,\lambda_1\lambda_2\lambda_3\begin{pmatrix} \lambda_1^{-1} & 0 & 0 \\ 0 & \lambda_2^{-1} & 0 \\ 0 & 0 & \lambda_3^{-1} \end{pmatrix} \tag{7.28}$$

$$= \begin{pmatrix} \mu\lambda_1 - \alpha\lambda_2\lambda_3 & 0 & 0 \\ 0 & \mu\lambda_2 - \alpha\lambda_1\lambda_3 & 0 \\ 0 & 0 & \mu\lambda_3 - \alpha\lambda_1\lambda_2 \end{pmatrix}\ . \tag{7.29}$$

Applying this to the uniaxial tension state considered above together with incompressibility yields

$$\boldsymbol{P} = \begin{pmatrix} \mu\,\lambda - \alpha\,\lambda^{-1} & 0 & 0 \\ 0 & \mu\,\lambda^{-1/2} - \alpha\,\lambda^{1/2} & 0 \\ 0 & 0 & \mu\,\lambda^{-1/2} - \alpha\,\lambda^{1/2} \end{pmatrix}\ . \tag{7.30}$$

The traction-free boundary conditions, $P_2 = P_3 = 0$, allow to determine the Lagrange multiplier, leading to $\alpha = \mu/\lambda$. Using the latter, one obtains $P = P_1 = \mu\,(\lambda - \lambda^{-2}) = \partial f/\partial\lambda$, as stated.

Example: Necking instabilities

Consider a bar of initial length ℓ_0 and cross-section s_0 that is stretched along its major axis by a tensile force of magnitude F, such that it features length ℓ and cross-section s. Suppose that the material is incompressible, i.e. that

$$s\ell = s_0\,\ell_0 \quad\Longrightarrow\quad s = s_0\frac{\ell_0}{\ell} = s_0\,e^{-\epsilon}\ , \tag{7.31}$$

where we used $\lambda = \ell/\ell_0 = e^{\epsilon}$. Consider then a tensile force F that stretches the bar, i.e.

$$F = s(\epsilon)\,\sigma(\epsilon) = s_0\,\sigma(\epsilon)\,e^{-\epsilon}\ . \tag{7.32}$$

This result shows that the response to the applied force F is composed of a constitutive part $\sigma(\epsilon)$ and a geometric part $s_0 \, e^{-\epsilon}$. We would like to understand the implication of this for various representative constitutive laws $\sigma(\epsilon)$. In a brittle material, e.g. window glass, we expect abrupt fracture at small ϵ as F is increased. We will discuss brittle fracture later in the course. Instead, let us consider materials that can be deformed to large deformation without breaking, i.e. metals and soft materials. Crystalline (metal) deformation will be discussed later in the course, but for our purposes here we note that metals usually exhibit a response that can be approximated as a power-law relation between stress and strain,

$$\sigma_{metal}(\epsilon) = E \, \epsilon^n \, , \tag{7.33}$$

where n is some positive power, typically smaller than unity. As a representative relation for soft materials, let us use the neo-Hookean law

$$\sigma_{nh}(\epsilon) = \mu \, (\lambda^2 - \lambda^{-1}) = \mu(e^{2\epsilon} - e^{-\epsilon}) \, . \tag{7.34}$$

Focus first on the case of a metal, in which we have

$$F_{metal} \sim \epsilon^n \, e^{-\epsilon} \, . \tag{7.35}$$

At small strains the constitutive power-law dominates the response, which is monotonically increasing, while at large strains the geometric term dominates the response, which is monotonically decreasing. In between, the response reaches a maximum at $\epsilon_c = n$. What are the mechanical implications of such a response? The existence of a peak force, $F_c \equiv F(\epsilon_c)$, above which there's no way to balance the force with a uniform deformation, implies an instability. In our case it takes the form of a necking instability where the bar's cross-section becomes smaller and smaller in some region, until the local stress is so large that the bar breaks. The necking instability is a typical mode of failure in metals under tension, as implied by our simple analysis. A complete account of the necking instability (initiation, critical wavelength, nonlinear evolution etc.) goes well beyond our simple analysis, which nevertheless gives us a sense of the phenomenon. What happens for the neo-Hookean material, say rubber? In this case we have

$$F_{rubber} \sim e^{\epsilon} - e^{-2\epsilon} \, , \tag{7.36}$$

which shows that the force is a monotonically increasing function of the strain. This suggests that there is no necking instability in this case. Indeed, soft materials (e.g. rubber) do not generally

undergo a necking instability under tension.

Example: Balloon (or blood vessel) under internal pressure

Consider a thin spherical shell made of an incompressible soft material (a balloon or a blood vessel. The latter may be more properly modelled as a cylindrical shell, but the results will be similar) under internal pressure of magnitude p. The internal radius in the undeformed (reference) configuration is L and the outer is $L + H$, with $H \ll L$. The corresponding quantities in the deformed configuration are ℓ and $\ell + h$. We also have $h \ll \ell$. This small parameter will be useful in solving the problem. Our goal is to determine the relation between the internal pressure and the deformation.

We can immediately write down the global stretches in this problem

$$\lambda_r = \frac{h}{H} \quad \lambda_\theta = \lambda_\phi = \frac{\ell}{L} \equiv \lambda . \tag{7.37}$$

Incompressibility implies (upon linearization with respect to h and H)

$$HL^2 \simeq h\ell^2 \quad \Longrightarrow \quad \frac{\ell}{L} = \sqrt{\frac{H}{h}} \quad \Longrightarrow \quad \lambda_r = \lambda^{-2} . \tag{7.38}$$

Consider then the force balance equation (r is the radial coordinate in the deformed configuration)

$$\partial_r \sigma_{rr} + \frac{2\sigma_{rr} - \sigma_{\theta\theta} - \sigma_{\phi\phi}}{r} = 0 . \tag{7.39}$$

The symmetry of the problem implies $\sigma_{\theta\theta} = \sigma_{\phi\phi} \equiv \sigma$. The boundary conditions read

$$\sigma_{rr}(r = \ell) = -p \quad \text{and} \quad \sigma_{rr}(r = \ell + h) = 0 , \tag{7.40}$$

where the minus sign in the first boundary condition ensures that the radial stress is compressive.

The radial stress varies in space, i.e. $\partial_r \sigma_{rr} \neq 0$. Since h is small, the boundary conditions imply that to leading order we have

$$\partial_r \sigma_{rr} \simeq \frac{p}{h} . \tag{7.41}$$

We then assume that $\sigma \gg p$ (we will check for consistency at the end) and hence Eq. (7.39) can be written as (where $r \simeq \ell$)

$$\frac{p}{h} - \frac{2\sigma}{\ell} \simeq 0 \quad \Longrightarrow \quad p \simeq \frac{2h\sigma}{\ell} \ll \sigma . \tag{7.42}$$

The last relation shows that our assumption about the relation between p and σ is valid (since $h \ll \ell$). Note that of course it was not necessary to a priori assume $\sigma \gg p$ and then check

for consistency a posteriori, though this procedure (i.e. of assuming something, exploring its implications and check for consistency at the end) is very common in theoretical physics and hence has a pedagogical/educational value. Alternatively, one can substitute $\sigma_{rr} \simeq -p$ in the force balance Eq. (7.39) and solving for p (we could use the spatial average of σ_{rr}, $-p/2$, but as we are interested in an order of magnitude estimate, it makes no difference), we obtain

$$p \simeq \frac{2h\sigma}{\ell\left(1 - \dfrac{2h}{\ell}\right)} \simeq \frac{2h\sigma}{\ell} + \mathcal{O}\left[\left(\frac{h}{\ell}\right)^2\right] , \tag{7.43}$$

which of course agrees with Eq. (7.42) to leading order in the smallness h/ℓ. It can be used to obtain higher order corrections (possibly with some additional considerations), but as $h/\ell \ll 1$, the leading order will be enough. Note that the spatial variation of σ_{rr} can be obtained from Eq. (7.41), together with the boundary condition at $r = \ell$, yielding

$$\sigma_{rr}(r) = \frac{p}{h}r - p\left(1 + \frac{\ell}{h}\right) . \tag{7.44}$$

We would now like to express p as a function of λ. Noting that

$$\frac{h}{\ell} = \frac{h}{H}\frac{H}{L}\frac{L}{\ell} = \frac{H}{L}\lambda^{-3} \tag{7.45}$$

we obtain

$$p(\lambda) \simeq \frac{2H}{L}\lambda^{-3}\sigma(\lambda) . \tag{7.46}$$

Again, we see that the response to the applied pressure p is composed of a constitutive part $\sigma(\lambda)$ (an increasing function) and a geometric part λ^{-3} (a decreasing function). The condition for the existence of a maximum in the response function reads

$$\frac{dp(\lambda_c)}{d\lambda} = 0 \implies \frac{d\sigma(\lambda_c)}{d\lambda} = \frac{3\sigma(\lambda_c)}{\lambda_c} , \tag{7.47}$$

which suggests an instability for $p > p(\lambda_c)$ occurring at the point where geometric thinning overcomes constitutive stiffening. As a concrete example, assume the material is neo-Hookean

$$f = \frac{\mu}{2}\left(\lambda_r^2 + \lambda_\theta^2 + \lambda_\phi^2 - 3\right) = \frac{\mu}{2}\left(2\lambda^2 + \lambda^{-4} - 3\right) , \tag{7.48}$$

which implies

$$\sigma(\lambda) = \lambda\frac{\partial f}{\partial \lambda} = 2\mu\left(\lambda^2 - \lambda^{-4}\right) \implies p(\lambda) \sim \lambda^{-1} - \lambda^{-7} . \tag{7.49}$$

Therefore, $\lambda_c = 7^{1/6} \simeq 1.38$. If a blood vessel experiences a pressure $p > p(\lambda_c)$, it might develop an aneurysm (which might be bad news).

Example: Elastic cavitation

Consider a spherical cavity of initial radius L inside an elastic material loaded by a radially symmetric tensile stress far away, σ^∞. The symmetry of the problem suggests that all quantities are functions of r alone and that $\sigma_{\phi\phi} = \sigma_{\theta\theta}$. The force balance equation reads

$$\partial_r \sigma_{rr} + 2\frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0 \ . \tag{7.50}$$

Integrating this equation from the deformed radius of the cavity ℓ to r we obtain

$$\sigma_{rr}(r) = -2 \int_\ell^r \frac{\sigma_{rr} - \sigma_{\theta\theta}}{\tilde{r}} d\tilde{r} \ , \tag{7.51}$$

where we used the traction-free boundary condition $\sigma_{rr}(r = \ell) = 0$ and $\tilde{r}$ is a dummy integration variable. Denote then $r' = \tilde{r}/\ell$ and focus on $r \to \infty$, we obtain

$$\sigma_{rr}(\infty) = -2 \int_1^\infty \frac{g(r', L/\ell)}{r'} dr' \ , \tag{7.52}$$

where $\sigma_{rr} - \sigma_{\theta\theta} = g(r', L/\ell)$ is a property of the solution (which involves also the constitutive relation). From our previous analysis we know that the existence of the cavity amplifies the (circumferential) stress at the surface as compared to the applied stress σ^∞ (for a cylindrical cavity we calculated the amplification factor to be 2 and for a sphere is it 3/2). If we keep on increasing the applied stress an ordinary material will simply break near the cavity surface. However, in soft materials something else can happen (the same can happen is an elasto-plastic material, to be discussed later). We can ask ourselves whether the cavity can grow (elastically!) without bound under the application of a finite stress at infinity. To mathematically formulate the question take the $\ell \to \infty$ limit in Eq. (7.52) and define

$$\sigma_c = -2 \lim_{\ell \to \infty} \int_1^\infty \frac{g(r', L/\ell)}{r'} dr' \ . \tag{7.53}$$

Therefore, if the integral above converges, then for any $\sigma^\infty > \sigma_c$ the cavity will grow indefinitely. The critical stress σ_c is called the cavitation threshold. σ_c is finite if $g(r', L/\ell) = \sigma_{rr} - \sigma_{\theta\theta} \to 0$ as $r \to \infty$, which is the typical situation.

Let us see how this works in a concrete example, where the goal is to find $\sigma_{rr} - \sigma_{\theta\theta} = g(r', L/\ell)$ and then evaluate the integral in Eq. (7.53). Consider an incompressible elastic material. As above, the initial radius of the cavity is L and the radial coordinate is denoted as R. The deformed radius is ℓ and the coordinate of the deformed configuration is r. Incompressibility

implies that the volume of any material piece in the reference configuration is conserved in the deformed one, in particular we have

$$\frac{4\pi}{3}\left(R^3 - L^3\right) = \frac{4\pi}{3}\left(r^3 - \ell^3\right) \quad \Longrightarrow \quad R(r) = (r^3 + L^3 - \ell^3)^{1/3} . \tag{7.54}$$

The non-radial stretches take the form

$$\lambda_\phi = \lambda_\theta = \frac{r}{R} . \tag{7.55}$$

Incompressibility implies

$$\lambda_r \equiv \lambda \quad \Longrightarrow \quad \lambda_\phi = \lambda_\theta = \lambda^{-1/2} \tag{7.56}$$

which leads to

$$\lambda^{-1/2} = \frac{r}{R} \quad \Longrightarrow \quad \lambda = \left(\frac{R}{r}\right)^2 . \tag{7.57}$$

Finally, this leads to

$$\lambda = \left(\frac{r^3 + L^3 - \ell^3}{r^3}\right)^{2/3} = \left[\frac{r'^3 + (L/\ell)^3 - 1}{r'^3}\right]^{2/3} , \tag{7.58}$$

with $r' \equiv r/\ell$. Consider then the stress state. It is triaxial and contains only the diagonal components $(\sigma_{rr}, \sigma_{\phi\phi}, \sigma_{\theta\theta})$, with $\sigma_{\phi\phi} = \sigma_{\theta\theta}$. However, since the material is incompressible we can superimpose on this stress state a hydrostatic stress tensor of the form $-\sigma_{\theta\theta}\boldsymbol{I}$ without affecting the deformation state, resulting in $(\sigma_{rr} - \sigma_{\theta\theta}, 0, 0)$, which is a uniaxial stress state in the radial direction. Therefore, the constitutive relation takes the form $\sigma_{rr} - \sigma_{\theta\theta} = g(\lambda_r)$. Focus then on a neo-Hookean material for which $g(\lambda) = \mu(\lambda^2 - \lambda^{-1})$ and evaluate the integral in Eq. (7.53)

$$\sigma_c = -2 \lim_{\ell \to \infty} \int_1^\infty \frac{g[\lambda(r', L/\ell)]}{r'} dr' = -2\mu \int_1^\infty \left[\frac{(1 - r'^{-3})^{4/3} - (1 - r'^{-3})^{-2/3}}{r'}\right] dr' . \tag{7.59}$$

This integral can be readily evaluated (just use $x \equiv 1 - r'^{-3}$ and $dx = 3r'^{-4}dr'$), yielding

$$\sigma_c = \frac{5\mu}{2} . \tag{7.60}$$

This result, which was verified experimentally (see, for example, J. Appl. Phys. **40**, 2520 (1969)), clearly demonstrates the striking difference between ordinary and "soft" solids. The *ideal* strength of ordinary solids is about $\mu/10$. The actual strength is *much* smaller (see later in the course). However, "soft" solids can sustain stresses larger than μ without breaking (though, as we have just shown, they can experience unique instabilities such as elastic cavitation).

C.   Small amplitude waves in nonlinear elastic solids

Let us consider now the propagation of elastic waves in nonlinearly elastic materials. We would like to focus on small amplitude waves that propagate on top of a nonlinearly deformed state. What would be the propagation speed of such waves?

To qualitatively address this issue we focus on a 1D formulation in which the constitutive law can be written as $\sigma(\epsilon)$. If the material is undeformed, then the constitutive law takes the form $\sigma = E\epsilon$ and waves propagate at a speed $\sqrt{E/\rho_0}$, where ρ_0 is the mass density in the undeformed configuration. Suppose now that material is already deformed to a strain ϵ (and hence experiences a stress $\sigma(\epsilon)$). The transport of energy and momentum at this state is still controlled by small amplitude elastic waves. The question is then, what elastic modulus determines the propagation speed? For that aim we define the tangent modulus as

$$E(\epsilon) = \frac{d\sigma}{d\epsilon} \ . \tag{7.61}$$

This modulus is a constant for linear elastic materials, but varies with the state of deformation for nonlinear elastic materials. The wave propagation speed would then be $\sqrt{E(\epsilon)/\rho(\epsilon)}$, where both the relevant modulus and the mass density depend on the current state of deformation through ϵ. We thus conclude that wave propagation in nonlinear elastic solids depends on the state of deformation which affects both the elastic constants and the mass density in the material framework. As usual, such calculations are much more convenient to perform in the reference configuration.

VIII.   SPATIOTEMPORAL INSTABILITIES

Spatiotemporal instabilities play an essential role in shaping the world around us. Practically all of the symmetry-breaking patterns observed in nature are generated by instabilities. The most generic approach to instabilities is known as linear stability analysis. The philosophy is simple; consider a set of partial differential equations, generically nonlinear, for a set of fields (schematically denoted by $f(\boldsymbol{x}, t)$)

$$\mathscr{D}\left[f(\boldsymbol{x}, t)\right] = 0 \ . \tag{8.1}$$

Suppose f_0 is a space- and time-independent (or steadily propagating) solution satisfying the global symmetries of a given problem (not always such solutions exist, see below). Introduce then a small spatiotemporal perturbation $\delta f(\boldsymbol{x}, t)$ such that

$$f(\boldsymbol{x}, t) = f_0 + \delta f(\boldsymbol{x}, t) \ . \tag{8.2}$$

Since δf is small compared to f_0, we can linearize the equations with respect to the small perturbation δf to obtain

$$\mathscr{L}\left[\delta f(\boldsymbol{x}, t)\right] = 0 \ . \tag{8.3}$$

Finally, we consider each Fourier mode separately

$$\delta f(\boldsymbol{x}, t) \sim e^{i \boldsymbol{k} \cdot \boldsymbol{x} + \omega t} \ , \tag{8.4}$$

where $\boldsymbol{k}$ is the spatial wavenumber and ω is the temporal frequency. The linearized Eqs. (8.3) then become algebraic equations for $\omega(\boldsymbol{k})$. Whenever $\Re\left[\omega(\boldsymbol{k})\right] > 0$, an instability is implied as the perturbation grows exponentially in time. Note that in many problems f_0 is a steadily propagating solution of the coordinate $\xi = x - c\,t$, in which case the formalism is applicable once ξ is used. In other problems, a time-independent solution $f_0(\boldsymbol{x})$ exists, in which case translational invariance is broken and not all wavenumbers $|\boldsymbol{k}|$ admissible. Finally, there are problems in which there exist no time-independent solutions (e.g., in the necking problem briefly discussed above, the spatially-homogeneous solution is intrinsically time-dependent, $f_0(t)$), in which case things become more complicated.

Linear stability analysis is a very useful tool, but it is also limited to some extent. Not finding a linear instability does not mean there exists no nonlinear one, or alternatively, finding a linear instability does not tell us what happens when the perturbation grows and nonlinearities intervene. To understand how this general framework works in a problem where elasticity plays

a central role (yet not an exclusive one), let us consider a concrete example.

Example: The Asaro–Tiller–Grinfeld (ATG) instability

Consider a solid, say of rectangular shape, under the application of a uniaxial tension (or compression) of magnitude σ_0 (the non-hydrostatic conditions are important). The stress is small and the response is linear elastic. The solution is simply that of homogeneous stress and it is stable (i.e. , if a compressive stress is applied, we assume the conditions for buckling are not met).

We now introduce a new (non-elastic, non-equilibrium) piece of physics: mass transport along the surface of the solid. The surface evolves with a normal velocity v_n, which is driven by variation of the chemical potential density μ (the chemical potential is the relevant thermodynamic quantity because we are talking about mass transport). Mathematically speaking we say that

$$v_n = \mathscr{D}(\mu) \,, \tag{8.5}$$

where $\mathscr{D}(\cdot)$ is a differential operator that depends on the physical nature of the mass transport We may think of several mass transport processes. When the solid is in equilibrium with its liquid phase (or gaseous phase), mass transport can take place by melting-recrystallization (or evaporation-condensation). In both cases, the transport law takes the form

$$v_n \sim -\Delta\mu \,, \tag{8.6}$$

where $\Delta\mu = \mu_s - \mu_l$ is the chemical potential difference between the solid and liquid phase (or gaseous phase μ_g). Another possible process would be surface diffusion, which is the surface analog of ordinary bulk diffusion. In this case, surface gradients of μ drive a material flux J_s

$$J_s \sim -\frac{\partial\mu}{\partial s} \,, \tag{8.7}$$

where s is the arclength parameterization of the surface. Mass conservation implies

$$v_n \sim -\frac{\partial J_s}{\partial s} \sim \frac{\partial^2\mu}{\partial s^2} \,. \tag{8.8}$$

Putting the prefactors in, we end up with

$$v_n = \frac{D}{\gamma}\frac{\partial^2\mu}{\partial s^2} \,, \tag{8.9}$$

where D, whose dimension is length^4/time, is proportional to the surface diffusion coefficient and γ is the surface tension. We stress that the evolution of the surface, encapsulated in v_n is a non-equilibrium dissipative process.

The next step would be to write down an expression for the chemical potential density (in the presence of a liquid phase, we are of course interested in the chemical potential difference between the solid and the liquid). Let us first write down the answer and then try to understand its origin. The chemical potential density contains two contributions, one is an elastic strain energy contribution near the surface and the other is a surface contribution

$$\mu = \mu_e + \mu_s = \frac{1 - \nu^2}{2E} (\sigma_{tt} - \sigma_{nn})^2 + \gamma\kappa \ , \tag{8.10}$$

where μ_e and μ_s are the elastic and surface energy contributions to the chemical potential density. t and n are the tangent and normal to the surface, respectively, γ is the surface tension/energy as above and κ is the surface curvature. If the surface is not in contact with its liquid phase, i.e. $\sigma_{nn} = 0$ (note that $\sigma_{nt} = 0$ with or without a liquid), the elastic contribution is simply the elastic strain energy in the solid. If the surface is in equilibrium with its liquid phase, then there is a finite pressure of magnitude $|\sigma_{nn}|$ also in the liquid, and the chemical potential difference depends on the difference $\sigma_{tt} - \sigma_{nn}$. This result also shows that under hydrostatic conditions in the solid, $\sigma_{tt} = \sigma_{nn}$ there's no elastic contribution (and the effect we are interested will disappear).

What about the surface energy contribution? The change in the Gibbs free energy due to surface area changes is $dG = \gamma dA$. Since the (surface) chemical potential is the change of G with the number of particles of total volume dV added to the surface, $\mu = dG/dV$, we should ask ourselves how the surface area changes when we add a volume dV of material to a surface (we stress that dV is not an incremental deformation, but rather represents a piece of a material). That obviously depends on the curvature of the surface. For a convex/concave surface an addition of a particle of volume dV results in an increase/decrease in the surface area by an amount $dA \sim dV\kappa$, where κ is the signed curvature (assumed positive for convex surfaces). To make this absolutely clear, consider a spherical surface of radius R and the addition of an infinitesimal mass element of volume dV. The change in the sphere's volume is given by $4\pi R^2 dR = dV$, and hence the change in the effective radius is $dR = dV/4\pi R^2$. Hence, the change is the area is $dA = d(4\pi R^2) = 8\pi R dR = 2dV/R \sim dV\kappa$. For a spherical cavity, we get the same result with a minus sign. Therefore, the surface energy contribution to the chemical potential density is $\gamma\kappa$.

Plugging the expression for μ in Eq. (8.10) into Eq. (8.9) we obtain a dynamic equation that can be used to study the stability of the surface against small perturbations. To be absolutely clear about the last point, we denote the deviation of the surface from being flat by $h(x,t)$, where x is the load application direction. Both v_n and μ can be expressed in terms $h(x,t)$. For a flat surface, $h(x,t) = 0$, $\kappa = 0$ and μ is constant $\mu = \frac{1-\nu^2}{2E}\sigma_0^2$ (here $\sigma_0 = \sigma_{tt} - \sigma_{nn}$). This, of course,

implies $v_n = 0$, as expected. To understand what happens when the surface is not flat, we should introduce a small spatiotemporal perturbation $h(x, t) \neq 0$ and see if it grows or decays in time. Before we do that, let us first try to make a rough estimate. For that aim, consider a square wave perturbation of the surface, with an amplitude a and a wavelength λ. Let us estimate the change in the Gibbs free energy due to the perturbation. On the one hand, the protruding parts of the perturbation are far less stressed than they were when the surface was flat. Therefore, the elastic energy (per wavelength) is reduced roughly by

$$\Delta G_e \sim -\frac{\sigma_0^2}{2E} \frac{\lambda a}{2} \ . \tag{8.11}$$

The surface energy is increased due to the creation of new surface of size $2a$ (again per wavelength) by

$$\Delta G_s = 2\gamma a \ . \tag{8.12}$$

Therefore, the total variation of the Gibbs free energy is given by

$$\Delta G = \Delta G_e + \Delta G_s \sim -\frac{\sigma_0^2}{2E} \frac{\lambda a}{2} + 2\gamma a \ . \tag{8.13}$$

The important insight here is that there is a competition between an elastic effect, that tends to reduce the free energy (a destabilizing effect), and a surface effect that tends to increase it (a stabilizing effect). For sufficiently small wavelengths, the surface term penalizes more, and stability is expected. For sufficiently large wavelengths, the elastic term wins and the free energy is reduced. The critical wavelength scales as

$$\lambda_c \sim \frac{\gamma E}{\sigma_0^2} \ , \tag{8.14}$$

where wavelengths satisfying $0 < \lambda < \lambda_c$ are stable and $\lambda > \lambda_c$ are unstable. While this is a crude estimate, it gives us some insight into the physics behind the instability and essentially the right answer (as we will see soon). Actually it is no more than a dimensional analysis, which is in general quite a powerful tool.

Let us now perform the analysis in a more systematic way, where our goal is to express the equation of motion for the surface to leading order in the deviation $h(x, t)$ from a flat surface. As we consider small shape perturbations of the surface and we limit ourselves to a linear analysis, this small perturbation can be always decomposed into a sum of Fourier modes. Hence, we can focus on each mode separately and write

$$h(x, t) = h_0 \, e^{ikx + wt} \ . \tag{8.15}$$

The small parameter in the problem is kh_0, i.e. we assume small surface gradients. We will linearize the equations with respect to this small parameter. To linear order the curvature reads

$$\kappa \simeq -\frac{\partial^2 h}{\partial x^2} , \tag{8.16}$$

which leads to

$$\mu_s \simeq \gamma k^2 h . \tag{8.17}$$

As expected, the surface term plays a stabilizing role for all k-vectors. The perturbed elastic problem is not very difficult to solve (you will be doing this in a tutorial session) and the result is

$$\sigma_{tt} - \sigma_{nn} \simeq \sigma_0 \left(1 - 2|k|h\right) . \tag{8.18}$$

Convince yourself that the k-space operator is a long-range elastic operator in real space, as expected from elastic interactions. The last result implies the following linearized expression

$$\mu_e \simeq \frac{(1-\nu^2)\sigma_0^2}{2E} \left(1 - 4|k|h\right) , \tag{8.19}$$

which indeed shows that elasticity plays a destabilizing role for all k-vectors. Therefore, as we obtained from the simple estimate above, there is a competition between a stabilizing surface effect and a destabilizing elastic effect. This is a generic situation when dealing with instabilities. Combining the two contributions, we obtain

$$\mu = \mu_e + \mu_s \simeq \frac{(1-\nu^2)\sigma_0^2}{2E} - \frac{2(1-\nu^2)\sigma_0^2}{E}|k|h + \gamma k^2 h . \tag{8.20}$$

In addition, we note that to linear order we have

$$v_n \simeq \frac{\partial h}{\partial t} . \tag{8.21}$$

For an evaporation-condensation/melting-recrystallization mass transport process (for which $\partial_t h \sim -\Delta\mu\{h\}$), we obtain the following dispersion relation

$$\omega(k) \sim \frac{2(1-\nu^2)\sigma_0^2}{E}|k| - \gamma k^2 . \tag{8.22}$$

For a surface-diffusion mass transport process (for which $\partial_t h \sim \partial_{xx}\mu\{h\}$ — note that to linear order $\partial_{ss} \simeq \partial_{xx}$), we obtain the following dispersion relation

$$\omega(k) \sim k^2 \left[\frac{2(1-\nu^2)\sigma_0^2}{E}|k| - \gamma k^2\right] . \tag{8.23}$$

The relation $\omega(k)$, known as the stability/instability spectrum, contains all of the information regarding the linear stability of a given physical system. Having it at hand, we are now in a

position to decide about the stability conditions. It is clear that $\omega > 0$ implies instability (an exponential growth of the perturbation) and $\omega < 0$ implies stability (an exponential decay of the perturbation). Therefore, for both mass transport mechanisms, we find a critical wavenumber of the form

$$k_c = \frac{2(1 - \nu^2)\sigma_0^2}{\gamma E} \; , \tag{8.24}$$

which is identical to our scaling estimate above up to prefactors of order unity. For $k > k_c$ perturbations are stable and for $0 < k < k_c$ they are unstable. This result shows there is a continuous range of unstable modes. Which one of these will be observed experimentally (the instability is observed experimentally and in fact it is very important for various technological processes)?

To answer this question we should introduce the concept of the "fastest growing mode" (or "most unstable mode"), which refers to the mode that grows most strongly and hence will be the one to be observed. In this case, we obtain slightly different results for melting-recrystallization (mr) (or evaporation-condensation) and for surface-diffusion (sd), because their stability spectrum is different (though its zero crossing is the same)

$$k_m^{mr} = \frac{k_c}{2} \quad \text{and} \quad \omega_m \sim k_m^2 \; , \tag{8.25}$$

$$k_m^{sd} = \frac{3k_c}{4} \quad \text{and} \quad \omega_m \sim k_m^4 \; . \tag{8.26}$$

As we explained above, an unstable mode grows and eventually its amplitude invalidates the linearity assumption, necessitating the need for a nonlinear analysis. We would like to know, for example, whether the surface develops narrow grooves (cusps) that may lead to cracking (global failure of the sample) or the unstable processes saturates at a finite amplitude. Usually numerical analysis is needed in order to answer such questions. The instability was first discovered by Asaro and Tiller in 1972 and then independently rediscovered by Grinfeld in 1986. An experimental evidence for the instability can be found, for example, in Phys. Rev. B **46**, 13487–13495 (1992). Some results on the nonlinear evolution of the instability can be found, for example, in Phys. Rev. Lett. **82**, 1736–1739 (1999).

It is important to note that the ATG instability is a generic instability whose existence is independent of parameters (it only requires a non-hydrostatic stress state). In other physical systems, one may find that all wavenumbers are stable for some range of the control parameters, but not for others. The ATG instability is very important for various physical systems and processes. For example, it significantly affects Molecular Beam Epitaxy (MBE), which is a method

for thin-film deposition of single crystals (i.e. the deposition of a crystalline overlayer on a crystalline substrate), widely used in the semiconductor devices industry (e.g. for your cellphones and WiFi).

Finally, we stress again that while elasticity plays an essential role in the instability, i.e. a reduction in the stored elastic energy overcomes the surface tension contribution (those who are interested in elastic effects on surface physics in general, are advised to consult the following review paper, Surface Science Reports **54**, 157–258 (2004)), the surface corrugation is *not* an elastic deformation (bending), but rather a result of mass transport, i.e. an irreversible process. Such processes will be discussed in the rest of the course.

Irreversible processes: dissipative constitutive behaviors

Up until now we mainly discussed deformation processes that did not involve dissipation, i.e. we essentially focussed on elastic constitutive behaviors. In the second part of the course we will extensively discuss irreversible deformation processes, i.e. dissipative constitutive behaviors. This will allow us to gain a deeper understanding into the non-equilibrium physics of materials.

IX.   VISCO-ELASTICITY

Let us first consider experimental observations. Suppose we impose a constant small stress on a solid. An elastic solid will be nearly instantaneously deformed into a strain level determined by its elastic moduli. However, many solid materials (e.g. polymers) continue to accumulate strain on a much longer timescale, exhibiting a "creep" behavior. Alternatively, suppose we impose now a fixed small strain to a solid. An elastic solid will reach nearly instantaneously a state of constant stress. However, many solid materials exhibit long timescales stress relaxation under such conditions. Our goal in this section is to develop some understanding of these physical behaviors, which are termed visco-elastic.

A.   Viscous deformation

Before discussing visco-elasticity, we would like first to consider the simplest dissipative behavior. To see how it emerges consider then the second law of thermodynamics as expressed in the dissipation inequality in (4.38) and assume that the material of interest cannot store elastic energy at all, i.e. its internal energy density is a function of the entropy alone, $u(s)$, and $\boldsymbol{D}$ does not contain an elastic component. In this case $-\dot{u}$ balances $T\dot{s}$ and we obtain

$$\boldsymbol{\sigma} : \boldsymbol{D} \geq 0 \ . \tag{9.1}$$

The simplest way to satisfy this dissipation inequality under all circumstances is by using

$$\boldsymbol{\sigma} = 2\eta\boldsymbol{D} \ , \tag{9.2}$$

where $\eta \geq 0$ being the Newtonian (shear) viscosity (in fact $\boldsymbol{\sigma}$ and $\boldsymbol{D}$ here should be replaced by their deviatoric parts). Indeed, a material that does not deform elastically and its rate of deformation is linearly related to the stress is simply a Newtonian fluid (note that actually we

also assumed incompressibility above). From a mathematical point of view, the viscosity relation in Eq. (9.2) is analogous to Hooke's law since in both cases we linearly relate gradients of the basic field (displacement in linear elasticity and velocity in Newtonian fluid mechanics) to the stress (of course physically they are fundamentally different, one being non-dissipative and the other purely dissipative). This is why these constitutive laws are simple and useful (but also limited): they are, after all, linear perturbation/response approaches. Using the viscosity relation in Eq. (9.2) one can derive the well-known Navier-Stokes equations that properly describe Newtonian fluids under a wide range of conditions.

Why do we consider fluid viscosity if our main interest here is in solids? This is in fact a very deep question that is intimately related to the emergence of solidity/rigidity in noncrystalline materials and discussing it thoroughly goes well beyond the scope of this course (we will nevertheless spend time discussing some basic aspects of this important issue). Having said that, we can still provide good answers to this question in the present context: (i) Many solids exhibit a viscous component in their mechanical response (though, of course, not an exclusively viscous response as Newtonian fluids) (ii) Considering viscous dissipation may allow us to gain some insight into the origin of dissipation in solids.

First, it would be good to have some numbers in mind. The shear viscosity of water (room temperature, low frequencies) is 10^{-3} Pa·sec. The shear viscosity of a glass at its glass temperature (in fact this is the operative definition of the glass temperature, but this is really another story) is 10^{12} Pa·sec. The viscosity of noncrystalline solids well below their glass temperature and of metals is extremely large, usually regarded as infinite.

At the beginning of this section we considered viscous deformation from a thermodynamic perspective. Let us adopt now a more microscopic approach to the viscous flow of fluids, with the hope of gaining some insight into dissipative deformation processes. When we apply a small stress to a crystalline solid interatomic distances vary as elastic energy is being stored, but atoms do not change their neighbors, i.e. they do not rearrange themselves into a new configuration in response to the applied stress. As we stressed earlier in the course, elastic deformation implies a memory of a single state/configuration. What happens in the same situation in a fluid? In this case it would be more illuminating to consider the application of a constant strain rate. If it were an elastic solid then the stress would increase in proportion to the applied strain rate (but not indefinitely).

In a Newtonian fluid, however, elastic energy cannot be stored and hence the stress must relax

somehow. The microscopic process that mediates stress relaxation, and therefore viscous flow, is molecular rearrangements in which molecules change their neighbors, usually by hopping motion. So inelastic behavior involves configurational changes that mediate stress relaxation and energy dissipation. Note, of course, that when Newtonian fluids are considered, configurational changes take place constantly even in the absence of external driving forces, i.e. particles diffuse. To better understand this, think of the molecular/atomic forces that do not allow two molecules to easily come closer to one another and therefore resist rearrangements/hopping motion and the accompanying stress relaxation. Let us assign an energy barrier Δ to the rearrangement process (of course Δ actually characterizes the state of the whole system, irrespective of whether it corresponds to a local process or not). In equilibrium, the rate of barrier crossing (transition) is proportional $\tau_0^{-1} \exp\left(-\frac{\Delta}{k_B T}\right)$, where τ_0 is the molecular vibration time. This fundamental result is valid when $\Delta \gg k_B T$ and is usually associated with Arrhenius (1889), Eyring (1935) and Kramers (1940) (the last two went beyond the first by calculating also the prefactor). In the absence of external driving forces, forward and backward transitions are equally probable and hence while transitions constantly take place, there is no net flow (in fact, detailed balance is satisfied). However, particles perform random walk in space with a typical jump distance a of the order of a molecular distance a and a time unit $\tau \equiv \tau_0 \exp\left(\frac{\Delta}{k_B T}\right)$. Therefore, the diffusion coefficient is

$$D \sim \frac{a^2}{\tau} \; . \tag{9.3}$$

Let us go back now to the situation in which we apply a small stress to the fluid. In this case the barrier crossings would be biased in the direction of the applied stress, giving rise to macroscopic flow. Following the previous discussion, the resulting (shear) strain rate (considered here to be a signed scalar that corresponds to an applied signed shear stress σ) takes the form

$$\dot{\epsilon} \sim \frac{1}{\tau_0} \left[\exp\left(-\frac{\Delta - \Omega\sigma}{k_B T}\right) - \exp\left(-\frac{\Delta + \Omega\sigma}{k_B T}\right) \right] \; , \tag{9.4}$$

where the first term describes forward transitions and and other backwards ones, and Ω is a molecular volume of the order of a^3 (note that to avoid confusion with the diffusion coefficient, we denote here the rate of deformation by $\dot{\epsilon}$). The last relation can be rewritten as

$$\dot{\epsilon} \sim \frac{1}{\tau} \sinh\left(\frac{\Omega\sigma}{k_B T}\right) \; . \tag{9.5}$$

Note that this expression satisfies the required symmetry $\dot{\epsilon}(-\sigma) = -\dot{\epsilon}(\sigma)$, which ensures consistency with the second law of thermodynamics, i.e. $\sigma\dot{\epsilon} \geq 0$. Following Eq. (9.2), the Newtonian viscosity

is in fact defined as

$$\eta \equiv \lim_{\dot{\epsilon} \to 0} \frac{\sigma}{\dot{\epsilon}} \; . \tag{9.6}$$

Using the above expression for $\dot{\epsilon}$ we obtain

$$\eta \sim \frac{k_B T}{\Omega} \tau_0 \exp\left(\frac{\Delta}{k_B T}\right) \; . \tag{9.7}$$

This result provides some insight into the origin of fluid viscosity. It is a product of a temperature dependent quantity of stress dimensions, $k_B T/\Omega$, and a relaxation timescale $\tau_0 \exp\left(\frac{\Delta}{k_B T}\right)$ that depends on the underlying structure and molecular interactions, and temperature, through $\Delta/k_B T$. This result also gives us a sense of the origin of the large viscosity of solids. An obvious effect would be a large ratio $\Delta/k_B T$, which tends to exponentially increase the viscosity. In fact, another important effect was hidden in our derivation. In the expression for $\dot{\epsilon}$ in Eq. (9.4) there is in fact a multiplicative factor that represents the probability to find molecules that can undergo hopping motion, which for the case of fluids we assumed to be of order unity, i.e. each molecule (on average) contributes to the flow at each time interval. In disordered solids this probability is much small, giving rise to a large pre-factor in Eq. (9.7).

The major message we take from the discussion of fluid viscosity is that inelastic, dissipative, deformation involves configurational changes in the state of the deformation system and that this change is mediated by some form of stress relaxation induced by particles rearrangements. While the nature and properties of these configurational stress relaxation processes will vary from system to system (e.g. polymeric solids vs. metals), the basic idea remains valid. The physics of such configurational changes is usually described at the continuum level by coarse-grained internal state variables, which are in fact non-equilibrium order parameters (extension of ordinary order parameters in equilibrium statistical physics). These will be discussed later.

A corollary of the above discussion of fluid deformation/flow is a fundamental result in statistical physics that is worth mentioning. Putting together Eqs. (9.3) and (9.7) leads to

$$\eta \, D \sim k_B T \; , \tag{9.8}$$

which is the famous *Stokes-Einstein relation*. It is a paradigmatic example of a fluctuation-dissipation relation (here diffusion describes equilibrium fluctuations and viscosity describes non-equilibrium dissipation). Ordinary solids do not satisfy this relation.

B. Bringing linear viscous and elastic deformation together

The experiments we described at the beginning of this section clearly demonstrate that solids might exhibit a viscous component in their response. How do we account for this piece of physics? More precisely, how do we describe a response that is both elastic and viscous?

As usual, we start by making some simplifying assumptions. In short, we assume linearity as well as spatial and temporal homogeneity. Under these conditions, the most general linear relation between the stress $\boldsymbol{\sigma}$ and the strain $\boldsymbol{\varepsilon}$ reads

$$\sigma_{ij}(t) = \int_{-\infty}^{t} G_{ijkl}(t - t')\dot{\varepsilon}_{kl}(t')dt' \ . \tag{9.9}$$

(since the elastic part of the deformation is assumed to be linear, $\boldsymbol{\varepsilon}$ is an appropriate strain measure to describe elasticity. As we also consider viscous deformation, which can be large, we should use $\boldsymbol{\epsilon}$ as in the previous discussion of fluid viscosity. We arbitrarily chose the former here, but we should remember that the deformation can in fact be large). The tensor $\boldsymbol{G}$ is sometimes termed the stress relaxation modulus (it has the dimensions of stress). Note that $\boldsymbol{G}(t-t')$ vanishes for $t' > t$ due to causality, i.e. the stress at time t can only be affected by strain variations that took place at earlier times, $t' < t$. This is manifested by the choice of the upper integration limit in Eq. (9.9). For $\boldsymbol{G}(t) = \boldsymbol{\eta}\,\delta(t)$, we obtain a purely viscous behavior $\boldsymbol{\sigma} = \boldsymbol{\eta}\,\dot{\boldsymbol{\varepsilon}}$ (note that here $\boldsymbol{\eta}$ is a fourth order viscosity tensor). For $\boldsymbol{G}(t) = \boldsymbol{C}\,H(t)$ (here $H(t)$ is the Heaviside step function), we recover the elasticity relation $\boldsymbol{\sigma} = \boldsymbol{C}\,\boldsymbol{\varepsilon}$ of Eq. (5.6), where $\boldsymbol{\varepsilon}(0) = 0$ is assumed. In general, all of the viscoelastic properties of a material are contained within a single time-dependent tensor, which is a generalization of the elasticity tensor. From the mathematical structure of Eq. (9.9) we immediately see that $\boldsymbol{G}(t)$ is in fact the stress response to a step strain $\dot{\boldsymbol{\varepsilon}}(t) = \boldsymbol{\varepsilon}_0\,\delta(t)$ or equivalently $\boldsymbol{\varepsilon}(t) = \boldsymbol{\varepsilon}_0\,H(t)$. If such a measurement is performed and the stress response $\boldsymbol{\sigma}(t)$ is tracked, one can obtain $\boldsymbol{G}(t)$ following

$$\boldsymbol{G} = \boldsymbol{\sigma}\boldsymbol{\varepsilon}_0^{-1} \ . \tag{9.10}$$

In a simple shear setting (for an isotropic material), we obtain $G(t) = \sigma(t)/\varepsilon_0$. Likewise, we can define a creep compliance modulus $\boldsymbol{J}$ that quantifies the response to a step stress as

$$\varepsilon_{ij}(t) = \int_{-\infty}^{t} J_{ijkl}(t - t')\dot{\sigma}_{kl}(t')dt' \ . \tag{9.11}$$

Note that as in Eq. (9.9), causality implies that the upper integration limit is t. In the scalar case and for a step stress $\sigma(t) = \sigma_0 H(t)$, we have

$$J(t) = \frac{\varepsilon(t)}{\sigma_0} \ . \tag{9.12}$$

While the creep compliance $J(t)$ (it has the dimensions of inverse stress) contains the same physical information as the stress relaxation modulus $G(t)$, transforming one into the other in the most general case is not necessarily trivial and might involve numerical evaluation of Fourier integrals. For a simple Newtonian fluid we have $J(t) = t/\eta$, while for an elastic solid we have $J(t) = H(t)/E$.

To get a better understanding of how visco-elasticity actually works, let us consider simple models. The basic elements that capture the linear visco-elastic response of solids are an elastic element (Hookean spring) whose response is given by

$$\sigma = E \, \varepsilon \, , \tag{9.13}$$

(we use here E as a representative elastic modulus, though the shear modulus μ can be used as well. The relevant modulus is determined by the properties of the loading, e.g. uniaxial vs. shear deformation) and a viscous element (dashpot) whose response is given by

$$\sigma = \eta \, \dot{\varepsilon} \, . \tag{9.14}$$

Any linear combination of these elements (connected in series or in parallel) describes a visco-elastic model. The complexity of the connected network of elements determines the complexity and richness of the model.

The Kelvin-Voigt model

One simple possibility would be connect a spring and a dashpot in parallel, i.e. to say that elastic deformation gives rise to an elastic stress σ^{el} and that viscous deformation gives rise to a viscous stress σ^{vis}, while both types of deformation share the same total strain ε. In this case, we have

$$\sigma = \sigma^{el} + \sigma^{vis} = E \, \varepsilon + \eta \, \dot{\varepsilon} \, . \tag{9.15}$$

This is known as the Kelvin-Voigt model. In fact, by substituting a step strain $\varepsilon(t) = \varepsilon_0 \, H(t)$ in the above equation we see that this model simply emerges as a sum of the elastic and viscous stress relaxation moduli

$$G^{KV}(t) = G^{el}(t) + G^{vis}(t) = E \, H(t) + \eta \, \delta(t) \, , \tag{9.16}$$

where the superscript 'KV' stands for Kelvin-Voigt. Let us calculate the creep compliance in this model. To that aim, we impose a step stress $\sigma(t) = \sigma_0 \, H(t)$ in Eq. (9.15). The initial strain

cannot jump (this would imply a diverging strain rate, which would imply an infinite viscous stress) and hence $\varepsilon(t{=}0) = 0$. Therefore, solving $\sigma_0 = E\,\varepsilon + \eta\,\dot{\varepsilon}$ with this initial condition yields

$$\varepsilon(t) = \frac{\sigma_0}{E}\left[1 - \exp\left(-\frac{Et}{\eta}\right)\right] \quad \Longrightarrow \quad J^{KV}(t) = \frac{\varepsilon(t)}{\sigma_0} = \frac{1}{E}\left[1 - \exp\left(-\frac{Et}{\eta}\right)\right] . \tag{9.17}$$

At short times, $t \ll \eta/E$ we have

$$J^{KV}(t) \simeq \frac{t}{\eta} , \tag{9.18}$$

i.e. a viscous response, while for long times, $t \gg \eta/E$, we have

$$J^{KV}(t) \simeq \frac{1}{E} , \tag{9.19}$$

which is an elastic response. Therefore, the Kelvin-Voigt model represents short timescales viscous response and long timescales elastic response, with a crossover at a characteristic time η/E. The existence of such a timescale is a qualitatively new physical feature that was absent in the elastic constitutive laws (where there exists no intrinsic timescale). The competition between elastic and viscous deformation gives rise to a characteristic timescale. In the creep compliance experiment, this corresponds to the typical time by which the system develops a strain of the order of σ_0/E. What happens if we remove the external stress, say at t', after the strain saturates (i.e. $t' \gg \eta/E$)? In this case, we set $\sigma = 0$ in Eq. (9.15) to obtain $0 = E\,\varepsilon + \eta\,\dot{\varepsilon}$, which is solved by

$$\varepsilon(t - t') = \frac{\sigma_0}{E}\exp\left[-\frac{E(t - t')}{\eta}\right] . \tag{9.20}$$

This implies that the Kelvin-Voigt model exhibits full recovery of the initial shape when the stress is removed after a constant deformation state has been reached. This might look like an elastic behavior, but it is not. Dissipation is involved.

The Maxwell model

Another simple model can be constructed by saying that the elastic and viscous response share the same stress σ, but contribute additively to the strain rate $\dot{\varepsilon}$, i.e.

$$\dot{\varepsilon} = \dot{\varepsilon}^{el} + \dot{\varepsilon}^{vis} = \frac{\dot{\sigma}}{E} + \frac{\sigma}{\eta} . \tag{9.21}$$

This model is known as the Maxwell model which corresponds to a spring and a dashpot connected in series. Let us see whether and how this model is consistent with the second law of thermodynamics. The dissipation inequality (for a scalar case) reads

$$\sigma\,\dot{\varepsilon} - \dot{u} + T\dot{s} \geq 0 . \tag{9.22}$$

Here again we treat u and s as quantities per unit volume. Unlike the purely viscous case, a visco-elastic solid can store elastic energy. The important point to note is that the internal energy density u cannot depend on the total strain ε, but rather on ε^{el}, $u = u(\varepsilon^{el}, s)$. There are deep reasons why the total strain cannot be regarded as an independent thermodynamic variable, but more importantly, we note that internal energy can be reversibly stored during deformation only through elastic strains and that stresses are always thermodynamically conjugate to these strains

$$\boldsymbol{\sigma} = \frac{\partial u}{\partial \boldsymbol{\varepsilon}^{el}} \ . \tag{9.23}$$

Therefore, $\dot{u} = \sigma\,\dot{\varepsilon}^{el} + T\dot{s}$, which leads to

$$\left(\sigma\dot{\varepsilon}^{el} + \sigma\dot{\varepsilon}^{vis}\right) - \left(\sigma\dot{\varepsilon}^{el} + T\dot{s}\right) + T\dot{s} \geq 0 \qquad \Longrightarrow \qquad \sigma\,\dot{\varepsilon}^{vis} \geq 0 \ . \tag{9.24}$$

This dissipation inequality is indeed satisfied by the choice $\sigma = \eta\,\dot{\varepsilon}^{vis}$, with $\eta \geq 0$. Note that in Eq. (9.24) the elastic power $\sigma\dot{\varepsilon}^{el}$ cancels out, i.e. the reversible part of the applied power is stored in the material (and accounted for in the internal energy), and of course does not contribute to the dissipation. This is precisely why the heat equation in Eq. (4.43) follows from Eq. (4.42) for elastically deforming materials.

Let us now consider the properties of the Maxwell model. By substituting a step stress $\sigma(t) = \sigma_0\,H(t)$ into Eq. (9.21) and integrating from $t' = 0^-$ to $t' = t$, we see that this model simply emerges as a sum of the elastic and viscous creep compliances

$$J^M(t) = J^{el}(t) + J^{vis}(t) = \frac{H(t)}{E} + \frac{t\,H(t)}{\eta} \ , \tag{9.25}$$

where the superscript 'M' stands for Maxwell. In this case, the short times, $t \ll \eta/E$, behavior is elastic

$$J^M(t) \simeq \frac{1}{E} \ , \tag{9.26}$$

while the long times, $t \gg \eta/E$, behavior is viscous

$$J^M(t) \simeq \frac{t}{\eta} \ . \tag{9.27}$$

Therefore, the Maxwell model represents short timescales elastic response and long timescales viscous response. This means that solids described by this model feature a finite Newtonian viscosity.

Let us calculate the stress relaxation modulus in the framework of this model. A step strain $\varepsilon(t) = \varepsilon_0\,H(t)$ is represented in this model by the initial condition $\sigma(t{=}0) = E\,\varepsilon_0$ (i.e. the spring

responds instantaneously, while the dashpot remains passive) for the equation

$$0 = \frac{\dot{\sigma}}{E} + \frac{\sigma}{\eta} , \tag{9.28}$$

valid for $t > 0$. The solution is readily obtained as

$$\sigma(t) = E\,\varepsilon_0 \exp\left(-\frac{Et}{\eta}\right) \quad \Longrightarrow \quad G^M(t) = \frac{\sigma(t)}{\varepsilon_0} = E\,\exp\left(-\frac{Et}{\eta}\right) . \tag{9.29}$$

As expected, in this case the material cannot support stresses on long timescales. What happens if during the stress relaxation process, say when the stress has reached a value $\sigma_1 < E\,\varepsilon_0$, all external constraints are being removed? In this case we have an instantaneous strain relaxation of magnitude σ_1/E, and the material remains deformed at a strain level of $\varepsilon_0 - \sigma_1/E$. The Maxwell model describes a simple, single timescale, exponential stress relaxation process. It is clear that both the Kelvin-Voigt and the Maxwell model may be too simple to capture a wide range of realistic visco-elastic phenomena. The limitations are quite clear: the Kelvin-Voigt model exhibits no short times elasticity and the Maxwell model exhibits no long times elasticity (which might be realistic for supercooled liquids and glasses near their glass transition temperature). These limitations are intrinsically related to the fact that these models involve only a single timescale. Real visco-elastic solids typically exhibit a range of timescales, which can be mathematically represented using the Maxwellian stress relaxation function as a Green's function by writing

$$G(t) = \int_\tau f(\tau)e^{-t/\tau}d\tau , \tag{9.30}$$

where $f(\tau)$ is a continuous distribution of response coefficients corresponding to different relaxation times τ. Since any visco-elastic model can be viewed as a combination of springs and dashpots, $f(\tau)$ represents a continuous distribution of such elements.

As we said above, the creep compliance $J(t)$ contains the same physical information as the stress relaxation modulus $G(t)$, though it is not trivial to explicitly transform one into the other in the most general case. Nevertheless, an implicit integral relation satisfied by these two functions can be obtained. It takes the form

$$\int_0^t G(t - t')J(t')dt' = t . \tag{9.31}$$

You will be asked to prove this relation in one of your homework assignments.

C.   Oscillatory response

In addition to stress relaxation and creep experimental protocols, one can also measure the visco-elastic response to an oscillatory perturbation. This experimental protocol is a fundamental

tool for probing the physics of visco-elastic materials. More generally, it is a standard way to probe the linear response of many physical systems and quantities (e.g. dielectric properties, mechanical properties etc.). In our context, we consider the application of a small amplitude periodic strain of the form

$$\varepsilon(t) = \varepsilon_0 e^{i\omega t} , \tag{9.32}$$

where as usual in linear response theory we use a complex representation (while physical quantities are represented either by the real part or imaginary one). We then track the stress response

$$\sigma(t) = \varepsilon_0 G^*(\omega) e^{i\omega t} , \tag{9.33}$$

where $G^*(\omega) = G'(\omega) + iG''(\omega)$ is the complex modulus. $G'(\omega)$ is known as the storage modulus and $G''(\omega)$ as the loss modulus (the physical meaning of these terms will become clear soon). If we scan over a wide range of angular frequencies ω, the function $G^*(\omega)$ can be determined. This function contains the same information as the stress relaxation modulus $G(t)$ (and hence also as the creep compliance modulus $J(t)$). To see this, substitute $\varepsilon_0 e^{i\omega t}$ in the scalar version of Eq. (9.9), yielding

$$\sigma(t) = \varepsilon_0 \int_{-\infty}^{t} i\omega G(t - t') e^{i\omega t'} dt' . \tag{9.34}$$

By a simple change of variables $\tilde{t} \equiv t - t'$ we obtain

$$G^*(\omega) = i\omega \int_0^\infty G(\tilde{t}) e^{-i\omega \tilde{t}} d\tilde{t} . \tag{9.35}$$

Therefore, the complex modulus $G^*(\omega)$ equals $i\omega$ times the unilateral Fourier transform of $G(t)$. Note that since $G'(\omega)$ and $G''(\omega)$ are derived from a single real function they are not independent. They are related by the Kramers-Kronig relations (to be discussed in a tutorial session). The Newtonian viscosity can be readily extracted according to

$$\eta = \lim_{\dot{\varepsilon} \to 0} \frac{\sigma}{\dot{\varepsilon}} = \lim_{\omega \to 0} \frac{G^*(\omega)}{i\omega} . \tag{9.36}$$

Let us apply this result to the Maxwell model, whose stress relaxation modulus $G^M(t) = E\exp(-Et/\eta)$ is given in Eq. (9.29). We then need to evaluate the following expression

$$\lim_{\omega \to 0} \frac{G^*(\omega)}{i\omega} = \lim_{\omega \to 0} \int_0^\infty G^M(t) e^{-i\omega t} dt . \tag{9.37}$$

In this case, but not necessarily always, we can exchange the order integration and the $\omega \to 0$ limit to obtain

$$\int_0^\infty G^M(t) dt = E \int_0^\infty e^{-Et/\eta} dt = \eta \int_0^\infty e^{-x} dx = \eta , \tag{9.38}$$

which confirms Eq. (9.36) for the Maxwell model.

The complex modulus can be also expressed as

$$G^*(\omega) = |G^*(\omega)|e^{i\delta(\omega)} \; , \tag{9.39}$$

where $G'(\omega) = |G^*(\omega)|\cos[\delta(\omega)]$, $G''(\omega) = |G^*(\omega)|\sin[\delta(\omega)]$ and

$$\tan[\delta(\omega)] = \frac{G''(\omega)}{G'(\omega)} \; , \tag{9.40}$$

which is known as the loss tangent. δ quantifies the phase shift between the perturbation (strain) and the response (stress). To understand the physics behind this terminology let us calculate the dissipation during one deformation cycle. We know that for an elastic solid this would give zero, i.e. no dissipation is involved, while for a viscous fluid all of the work is being dissipated. Let's see what happens in the case of a viscous-elastic solid. For that aim we would like to integrate the incremental work $\sigma d\varepsilon$ over a complete cycle

$$W_{dis} = \oint \sigma d\varepsilon \; . \tag{9.41}$$

We use $d\varepsilon = \Re[\dot{\varepsilon}dt] = -\omega\varepsilon_0\sin(\omega t)dt$ and $\sigma = \Re[\varepsilon_0|G^*|e^{i(\omega t+\delta)}] = \varepsilon_0|G^*|\cos(\omega t + \delta)$

$$W_{dis} = \oint \sigma d\varepsilon = -\varepsilon_0^2|G^*| \int_0^{2\pi/\omega} \omega \sin(\omega t)\cos(\omega t + \delta)dt = \pi\varepsilon_0^2|G^*|\sin\delta \propto G'' \; . \tag{9.42}$$

Therefore, we observe that in cyclic deformation a visco-elastic material dissipates energy in proportion to the loss modulus, hence the name. Furthermore, since the latter vanishes when $\delta = 0$, the term loss tangent becomes clear. In fact, one can show that $W_{dis}/W_{sto} \propto \tan\delta$, where W_{sto} is the stored energy (by the elastic component) in the first quarter-cycle (prove). Finally, let us calculate the complex modulus for the Kelvin-Voigt and Maxwell models. For the former we substitute $\varepsilon(t) = \varepsilon_0 e^{i\omega t}$ in Eq. (9.15) obtaining

$$\sigma(t) = \varepsilon_0(E + i\omega\eta)e^{i\omega t} \Longrightarrow G^*(\omega) = E + i\omega\eta \; . \tag{9.43}$$

Again, we see the same picture emerging, the response is viscous at high frequencies (short timescales) and elastic at low frequencies (long timescales). The storage and loss moduli are $G' = E$ and $G'' = \eta\omega$. For the Maxwell model we use Eq. (9.21) to obtain

$$G^*(\omega) = E\frac{\frac{i\omega\eta}{E}}{1 + \frac{i\omega\eta}{E}} \; . \tag{9.44}$$

The corresponding storage and loss moduli read

$$G'(\omega) = E\frac{\left(\frac{\omega\eta}{E}\right)^2}{1 + \left(\frac{\omega\eta}{E}\right)^2} \quad \text{and} \quad G''(\omega) = E\frac{\frac{\omega\eta}{E}}{1 + \left(\frac{\omega\eta}{E}\right)^2} \; . \tag{9.45}$$

The low frequency behavior is dominated by the viscous response $G''/E \sim \omega \gg G'/E \sim \omega^2$, while the high frequency behavior is dominated by the elastic response $G'/E \sim 1 \gg G''/E \sim \omega^{-1}$. In addition, note that 'low' and 'high' frequencies are defined relative to the characteristic frequency scale in the model, $\sim E/\eta$. As stressed above, in most cases these are oversimplified models, yet they provide us with some basic physical understanding.

D. Viscoelastic waves

An important application of visco-elastic materials is in energy absorbing devices, which are used as mechanical dampers. To get a feeling how this works (in principle, we are of course not considering the devices themselves), let us consider wave propagation through a visco-elastic material. We focus on a scalar case and write the displacement field as $u(x,t) = u^*(x,\omega)e^{i\omega t}$ and the stress field as

$$\sigma(x,t) = \sigma^*(x,\omega)e^{i\omega t} = G^*(\omega)\frac{\partial u^*}{\partial x}e^{i\omega t} \; , \tag{9.46}$$

where we used $\varepsilon(x,t) = \frac{\partial u(x,t)}{\partial x} = \frac{\partial u^*}{\partial x}e^{i\omega t}$. Substituting these expressions in the momentum balance equation

$$\frac{\partial \sigma}{\partial x} = \rho\frac{\partial^2 u}{\partial t^2} \; , \tag{9.47}$$

we obtain

$$G^*(\omega)\frac{\partial^2 u^*}{\partial x^2} = -\rho\omega^2 u^* \; . \tag{9.48}$$

Using $u^* \sim e^{-ikx}$, we obtain a propagating plane-wave solution of the form

$$u(x,t) \sim \exp\left[i\omega\left(-\sqrt{\frac{\rho}{G^*(\omega)}}x + t\right)\right] \; . \tag{9.49}$$

We observe that G^* plays the role of the elastic constant in an ordinary (elastic) plane wave and that $\sqrt{G^*(\omega)/\rho}$ is a complex wave-speed. Suppose we would like to transmit low frequency waves and strongly attenuate high frequency ones. What kind of a material do we need? We would like to have a strong dissipative (viscous-like) response at high frequencies and an elastic response at low frequency. Therefore, our material should be Kelvin-Voigt-like. Let us use the complex modulus of the Kelvin-Voigt model in Eq. (9.43) as an example

$$G^*(\omega) = E(1 + i\omega\tau) \; , \tag{9.50}$$

where $\tau = \eta/E$. We are interested in the inverse complex speed

$$\sqrt{\frac{\rho}{G^*(\omega)}} = \sqrt{\frac{\rho}{E}}\frac{1}{\sqrt{1 + i\omega\tau}} \equiv \frac{1}{c}\frac{1}{\sqrt{1 + i\omega\tau}} \ , \tag{9.51}$$

in the limits $\omega\tau \ll 1$ and $\omega\tau \gg 1$. In the low frequency limit, $\omega\tau \ll 1$, we have

$$\sqrt{\frac{\rho}{G^*(\omega)}} = \frac{1}{c}\frac{1}{\sqrt{1 + i\omega\tau}} \simeq \frac{1}{c}\left(1 - \frac{i\omega\tau}{2}\right) \ . \tag{9.52}$$

Substituting this result into Eq. (9.49) we obtain

$$u \sim \exp\left[-\frac{i\omega\,(x - c\,t)}{c}\right]\exp\left[-\frac{x}{\ell(\omega)}\right] \ . \tag{9.53}$$

Here

$$\ell(\omega) \equiv \frac{2c}{\omega^2\tau} \sim \frac{\lambda}{\omega\,\tau} \gg \lambda \qquad \text{for} \qquad \omega\,\tau \ll 1 \ , \tag{9.54}$$

where $\lambda = 2\pi c/\omega$ is the wavelength. Therefore, in the low frequency limit waves propagate at the ordinary wave speed with a large attenuation length scale ℓ (many wavelengths). This is expected as the Kelvin-Voigt model is predominantly elastic in the long timescales limit.

In the opposite limit, $\omega\tau \gg 1$, we have

$$\sqrt{\frac{\rho}{G^*}} = \frac{1}{c}\frac{1}{\sqrt{1 + i\omega\tau}} \simeq \frac{1 - i}{c\sqrt{2\omega\tau}} \ . \tag{9.55}$$

Substituting this result into Eq. (9.49) we obtain (defining $\tilde{\ell}(\omega) \equiv c\sqrt{2\omega\tau}/\omega$)

$$u \sim \exp\left[-\frac{ix}{\tilde{\ell}(\omega)} + i\omega\,t\right]\exp\left[-\frac{x}{\tilde{\ell}(\omega)}\right] = \exp\left[-i\frac{(x - \tilde{\ell}(\omega)\,\omega\,t)}{\tilde{\ell}(\omega)}\right]\exp\left[-\frac{x}{\tilde{\ell}(\omega)}\right] \ , \tag{9.56}$$

which shows that both the wavelength and the decay length are determined by $\tilde{\ell}(\omega)$ (which actually means that the wavelength is ill-defined). Hence we conclude that in the high frequency limit wave propagation is completely attenuated.

X.   THERMODYNAMICS WITH INTERNAL VARIABLES

The discussion of visco-elasticity above provides a framework, both mathematical and experimental, for describing the linear visco-elastic response of materials. The latter is encapsulated in response functions such as the stress relaxation modulus $G(t)$, the creep compliance modulus $J(t)$ or the complex modulus $G^*(\omega)$. While being very useful, these functions (e.g. $G(t)$ and $J(t)$, which are "memory functions") do not reveal the physics that underlie dissipation and memory. To better account for the underlying physics one needs to identify in each systems, or class of systems, the nonequilibrium degrees of freedom that are responsible for dissipation and memory — i.e. the account for the configurational/srucural changes in the material — and to write coarse-grained equation of motion for them.

This requires a new concept, that of internal state fields ("internal variables"). To see this, let us consider the viscous part of the strain rate (as in the Maxwell model, cf. Eq. (9.21)), $\dot{\boldsymbol{\epsilon}}^{vis}$, and write it in the form

$$\dot{\boldsymbol{\epsilon}}^{vis} = \dot{\boldsymbol{\epsilon}}^{vis}(\boldsymbol{\sigma}, T, ...) \ . \tag{10.1}$$

The "..." represents the "something else", related to the evolution of the material's structure, which we need to account for in addition to conventional thermodynamic fields such as $\boldsymbol{\sigma}$ and T. We replace the "..." by a (small) set of coarse-grained internal variables/field, which describe the structural state of the material and are a generalization of "order parameters" in equilibrium statistical thermodynamics. Formally, we denote the set of these internal variables by $\{\Lambda_\alpha\}$ and rewrite the above equation as

$$\dot{\boldsymbol{\epsilon}}^{vis} = \dot{\boldsymbol{\epsilon}}^{vis}(\boldsymbol{\sigma}, T, \{\Lambda_\alpha\}) \ . \tag{10.2}$$

Obviously a macroscopic system contains an extensive number of structural degrees of freedom. How then do we choose a *small* set of state variables? How do we coarse-grain? How do we derive evolution equations for the internal variables? How do we self-consistently integrate these internal variables into thermodynamics?

Instead of developing a general (and rather abstract) formalism that addresses these questions, we will follow here another path in which we develop these ideas following a concrete example. The example concerns the volume deformation of a material, which contains both elastic and dissipative parts, and is assumed to be macroscopically homogenous (i.e. we neglect spatial gradients etc.). Such volume deformation is visco-elastic, and hence will complement and extend the discussion in the previous part of the course. The example is sufficiently generic to be relevant

for the discussion of plastic deformation in the next part of the course. It is also simple enough to work out all of the details without mathematical complications and will teach us a lot.

The first step would be to decompose the elastic and viscous/dissipative parts of the rate of deformation as done in the Maxwell model

$$\dot{V} = \dot{V}^{el} + \dot{V}^{vis} \ . \tag{10.3}$$

Obviously the viscous/dissipative rate of deformation may depend on the pressure p and the temperature T. However, our main focus here is on internal variables, so we would like to ask ourselves how to relate irreversible volume deformation to the material's structure (the elastic part is of course described as usual by the bulk modulus and the thermal expansion coefficient). A natural assumption would be that irreversible volume deformation is mediated by the formation and annihilation of vacancies. A vacancy carries a "unit" of irreversible volume deformation of magnitude v_0. Therefore, $\dot{V}^{vis}$ can be written as

$$\dot{V}^{vis}(p, T, N_v) = \dot{V}^{vis} = v_0 \, \dot{N}_v \ , \tag{10.4}$$

where N_v is the number of vacancies and serves as our internal variable. Note that N_v is a dynamical variable that satisfies its own equation of motion. In addition, as N_v is a non-equilibrium thermodynamic variable that represents a macroscopic number of degrees of freedom, we should associate with it energy and entropy.

The next step would be to write down the laws of thermodynamics as

$$\dot{U} + \dot{U}_R = -p\dot{V} \ , \tag{10.5}$$

$$\dot{S} + \dot{S}_R \geq 0 \ . \tag{10.6}$$

Our system experiences a pressure p and is coupled to a thermal reservoir of temperature T_R. The reservoir degrees of freedom are denoted by the subscript R.

At this point we should discuss the entropy of the system S. Why does it deserve a special attention? The point is that the internal variable N_v may fall out of equilibrium with the applied pressure p and temperature T, and hence S should in fact be a non-equilibrium entropy. We define S as

$$S(U, V^{el}, N_v) = k_B \log \Omega(U, V^{el}, N_v), \tag{10.7}$$

where $\Omega(U, V^{el}, N_v)$ is a constrained measure of the number of states of the system with energy U, elastic volume V^{el}, and a specified value of the internal variable N_v. N_v is out of equilibrium

if its value is not the one that maximizes S. When it does maximize S, i.e. when $N_v = N_v^{eq}$, then we require that the equilibrium entropy $S_{eq}(U,V) = k_B \log \Omega(U,V)$ be accurately approximated by

$$\frac{1}{V} S_{eq}(U,V) \approx \frac{1}{V} S(U,V,N_v^{eq}). \tag{10.8}$$

This approximation must become an equality in the thermodynamic limit, $V \to \infty$. Note also that once N_v equilibrates, we no longer distinguish between the total volume and its elastic and viscous parts.

Next, we invert the entropy in favor of the internal energy $S(U, V^{el}, N_v) \to U(S, V^{el}, N_v)$ and as usual have

$$\left(\frac{\partial U}{\partial S}\right)_{V^{el}, N_v} = T , \quad \left(\frac{\partial U}{\partial V^{el}}\right)_{S, N_v} = -p. \tag{10.9}$$

Therefore,

$$\dot{U} = -p\,\dot{V}^{el} + \left(\frac{\partial U}{\partial N_v}\right)_{S, V^{el}} \dot{N}_v + T\,\dot{S} . \tag{10.10}$$

The first law then becomes

$$-p\,\dot{V}^{vis} - \left(\frac{\partial U}{\partial N_v}\right)_{S, V^{el}} \dot{N}_v - \dot{U}_R = T\,\dot{S}, \tag{10.11}$$

where we have used $\dot{V} = \dot{V}^{el} + \dot{V}^{vis}$ to eliminate $\dot{V}^{el}$. The quantity

$$W \equiv -p\,\dot{V}^{vis} - \left(\frac{\partial U}{\partial N_v}\right)_{S, V^{el}} \dot{N}_v , \tag{10.12}$$

is an important one. It quantifies the difference between the dissipative work and the rate of internal energy stored in the internal variable N_v, termed "the stored energy of cold work".

We then isolate $\dot{S}$ in the above version of the first law, $\dot{S} = (W - \dot{U}_R)/T$, and insert it into the second law to obtain

$$W - \left(1 - \frac{T}{T_R}\right) \dot{U}_R \geq 0, \tag{10.13}$$

where we used $\dot{S}_R = \dot{U}_R/T_R$ (i.e. the bath is assumed to be a "simple fluid" characterized by an internal energy of the form $U_R(S_R)$, or alternatively by $S_R(U_R)$). Since we can vary the reservoir energy U_R independently of N_v (which controls W), we can split the inequality above into two independent inequalities of the form

$$W = -p\,\dot{V}^{vis} - \left(\frac{\partial U}{\partial N_v}\right)_{S, V^{el}} \dot{N}_v \geq 0, \tag{10.14}$$

and

$$-\left(1 - \frac{T}{T_R}\right) \dot{U}_R \geq 0. \tag{10.15}$$

The first inequality stresses again that not all of the viscous power $-p\dot{V}^{vis}$ is dissipated, i.e. that part of it is stored in the structural degrees of freedom which evolve with irreversible deformation. The second inequality is satisfied by requiring that $\dot{U}_R$ be a function of T that changes sign only when $T = T_R$; therefore we write

$$-\dot{U}_R = A\,(T_R - T) \equiv Q, \tag{10.16}$$

where $A \geq 0$ and Q is the rate at which heat is flowing into the system from the reservoir. It is important to understand that even if we make the common assumption of very strong heat coupling between the reservoir and the system, $A \to \infty$, Q remains finite. This simply means that in this limit $T \to T_R$ (as we expect) such that the product $A\,(T_R - T)$ is finite. Note also that Eq. (10.16) involves an equality, not an inequality. With this definition of Q, Eq. (10.11) becomes

$$C_v\dot{T} \simeq T\,\dot{S} = W + Q = W + A\,(T_R - T)\,, \tag{10.17}$$

where C_v is the heat capacity. This is a heat equation, which is driven by two terms. One is the coupling to the heat reservoir, which tends to equilibrate T with T_R. The strength of the coupling is $A \geq 0$ (we usually assume this coupling to be large). The other is the dissipation associated with viscous deformation, which is a source term that tends to heat the system. This is a very general result (in a spatially varying situation an additional diffusion term would appear as well).

Our next and important task is to calculate the dissipation term W. For that aim, we need to associate energy and entropy with the internal variable N_v. We then write

$$U(S, V^{el}, N_v) = U_0(N_v) + U_1(S_1) + U_{el}(V^{el}) = e_0\,N_v + U_1\big[S - S_0(N_v)\big] + U_{el}(V^{el}). \tag{10.18}$$

Here $U_0(N_v)$ is the energy of the vacancies, e_0 is the formation energy of a vacancy, $S_0(N_v)$ is the entropy of the vacancies $U_{el}(V_{el})$ is the elastic energy, and S_1 and U_1 are, respectively, the entropy and energy of all of the other degrees of freedom in the system. Equivalently, we can invert this relation and write it as an expression for entropy S

$$S(U, V^{el}, N_v) = S_0(N_v) + S_1(U_1) = S_0(N_v) + S_1\big[U - e_0\,N_v - U_{el}(V^{el})\big]. \tag{10.19}$$

The structure of these relations, i.e. the arguments of U_1 and S_1 in their second versions, describes the way the energy and entropy are shared between the vacancies and the other degrees of freedom. Note that the total entropy and energy in Eqs. (10.18)-(10.19) are assumed to have very simple forms.

We then assume that the vacancy population is dilute, i.e. that $N_v \ll N$ (where N is the number of available sites, proportional to the number of particles in the system), and therefore

$$S_0(N_v) \simeq k_B \left[- N_v \log \left(\frac{N_v}{N} \right) + N_v \right] , \tag{10.20}$$

which is of course extensive. (Just to remind you how to derive this result: The number of ways to distribute N_v objects among N sites is give by $\Omega = \frac{N!}{N_v!(N-N_v)!}$. Take the logarithm, invoke Stirling's approximation, i.e. $\log(x!) \simeq x \log x - x$ for large x, and $N_v \ll N$.). Note that

$$\frac{\partial S_0}{\partial N_v} = k_B \frac{\partial}{\partial N_v} [N_v \log N - N_v \log N_v + N_v] = -k_B \log \left(\frac{N_v}{N} \right) . \tag{10.21}$$

Finally, we are able to calculate W for which we need first to evaluate

$$\left(\frac{\partial U}{\partial N_v} \right)_{S,V^{el}} = \frac{\partial}{\partial N_v} [U_0(N_v) - T S_0(N_v)] = e_0 + k_B T \log \left(\frac{N_v}{N} \right) . \tag{10.22}$$

This leads to

$$W = -p v_0 \dot{N}_v - \left[e_0 + k_B T \log \left(\frac{N_v}{N} \right) \right] \dot{N}_v \equiv - \left(\frac{\partial G_v}{\partial N_v} \right)_{T,p} \dot{N}_v \geq 0 , \tag{10.23}$$

where

$$G_v = e_0 N_v - T S_0(N_v) + p v_0 N_v \tag{10.24}$$

is a vacancy-related Gibbs free-energy (it has the structure "$U - TS + pV$"). To satisfy the second law inequality in (10.23), we demand that both $-\partial G_v/\partial N_v$ and $\dot{N}_v$ change sign at the same point. G_v attains a minimum at $N_v = N_v^{eq}$ determined by

$$\left(\frac{\partial G_v}{\partial N_v} \right)_{T,p} = 0 \quad \Longrightarrow \quad N_v^{eq}(p,T) = N \exp \left(-\frac{e_0 + p v_0}{k_B T} \right) . \tag{10.25}$$

The equilibrium number of vacancies is determined by the vacancy enthalpy $e_0 + p v_0$ through a Boltzmann factor. We then conclude that $-\partial G_v/\partial N_v$ is a monotonically decreasing function that changes sign at N_v^{eq}. The inequality in (10.23) is satisfied if $\dot{N}_v$ has the same property. It is crucial to note that in principle we have not assumed any special proximity to equilibrium and hence the deviation of N_v from N_v^{eq} need not be small, going beyond linear response. However, the degree of non-linearity is a matter of physics, not of thermodynamics, and should emerge from more detailed physical considerations. For example, in the linear response regime the inequality in (10.23) can be satisfied by a linear relation of the form

$$\dot{N}_v = \Gamma(T, N_v) \left(N_v^{eq}(p,T) - N_v \right) , \tag{10.26}$$

where $\Gamma(T, N_v)$ a positive rate factor. A nonlinear model, which we do not work out here, may lead to

$$\dot{N}_v \sim -N_v \log \left(\frac{N_v}{N_v^{eq}} \right) \ .$$
(10.27)

The point is clear: any physical model should be consistent with the inequality in (10.23). It is important to note that the rate factor (i.e. the proportionality factor which has the dimension of inverse time) also contains essential physics that goes beyond thermodynamics. For example, if it deviates from a constant molecular rate – it can be much smaller and actually depend by itself on N_v — we can obtain interesting "slow" dynamics.

The upshot of this analysis are the evolution equations for T and N_v. The latter can be used to obtain $\dot{V}^{vis}$ and once a thermo-elastic energy functional is specified, the volume $V(t)$ can be calculated for any prescribed loading $p(t)$ and reservoir temperature $T_R(t)$.

The example we worked out in detail was quite simple. Usually, things are much more involved. The basic structure of the non-equilibrium thermodynamic theory, however, and the concepts discussed are rather general.

XI.   THE EMERGENCE OF SOLIDITY: AMORPHOUS SOLIDS AND THE GLASS TRANSITION PUZZLE

It would be impossible to discuss the physics of solids without mentioning the glass transition puzzle. The question that we ask first is how do solids form (in fact, we actually ask what is a solid)? The simple textbook answer is that solids form through a crystallization process, which is a first-order phase transition, as their liquid phase is cooled below the melting temperature T_m. However, a substantial fraction of the solids around us are not crystalline or polycrystalline. Think of your window glass or of a piece of plastic. They are amorphous solids. How do they form? When we mentioned the first-order phase transition through which crystals are formed, we did not refer to the dynamical aspects of the process. Being a first-order phase transition, the crystallization process requires the nucleation of a critical crystalline nucleus within the liquid. This nucleation process is stochastic, has a finite free-energy activation barrier and is driven by thermal fluctuations. It takes a finite time to be activated and it depends exponentially on the temperature. Therefore, for the phase transition to take place we need to cool the liquid sufficiently slowly through its melting temperature T_m. If, on the other hand, we do it faster, the phase transition does not take place. What happens then?

Consider a thermodynamic quantity, say the volume or the enthalpy, and plot it as a function of the temperature T for different cooling rates. For sufficiently small rates a first-order phase transition occurs at $T = T_m$, accompanied by a sharp drop in the thermodynamic quantity. A crystal is formed. As we explained above, when the cooling rate is sufficiently increased, there is no phase transition and the curve continues to go down smoothly with the decreasing temperature. A supercooled liquid is born. Supercooled liquids are meta-stable equilibrium states. At some point, near a temperature that is termed the "glass temperature" T_g, the curve levels off. A glass (an amorphous solid) is born. What is the nature of this state of matter? To start scratching the surface of this fascinating branch of physics, let us consider another macroscopic variable, the Newtonian viscosity. As we said above (in our discussion of visco-elastic solids), the Newtonian viscosity of ordinary liquids, say water (at room temperature), is 10^{-3} Pa·sec. Let us now plot the logarithm of the Newtonian viscosity η as a function of $1/T$ (it is called an Arrhenius plot). For simple liquids (as we discussed above), we expect this curve to be a straight line. This is true at high temperatures. However, when the temperature approaches the glass temperature T_g a dramatic (strongly nonlinear) increase of the viscosity is observed. We are talking about 10 orders of magnitude within a narrow window of temperatures. This is one of the most dramatic

phenomena we know of in terms of dynamical range. However, as far as we know, there is no phase transition (i.e. no divergence or singularity) in this range of temperatures. The viscosity curve is smooth. What then is the glass temperature T_g? It is operatively defined as the temperature for which the viscosity reaches 10^{12} Pa·sec. At this high level of viscosity a shear stress can be sustained by the glass for a macroscopic time, of about 10^2 sec (this is 14 orders of magnitude larger than the microscopic timescale, which is of the order of picoseconds). When the temperature is further reduced, the viscosity shoots up so strongly that the glass can sustain shear stresses for extremely long timescales, effectively infinite. For example, Plexiglass or Polycarbonate (i.e. the material from which your eye-glasses are made) are at about $0.7 - 0.8T_g$ (at room temperature) and you were never worried that they would start flowing.

To better appreciate these effects, let us briefly mention the Pitch drop experiment, the longest scientific experiment ever. It was initiated in 1930 at the University of Queensland, Australia. The experimental configuration consists of Pitch (a glassy polymer) which is allowed to flow under gravity through a funnel. The Pitch viscosity is estimated to be 10^{11} times larger than that of water (i.e. it is above its T_g) and since then only 9 drops have fallen and the tenth is currently forming. During the years in which the Pitch has been dripping no one has ever seen a drop falls. If you want to try your luck, you can visit: http://smp.uq.edu.au/content/pitch-drop-experiment, where the experiment is continuously broadcast online.

Correlation functions, fluctuations, α relaxation times and stretched exponentials

The crucial question, which is still regraded as one of the biggest puzzles in condensed-matter physics, statistical physics and materials science, is what makes a glass a solid, i.e. how come it can sustain a shear stress for enormously large times? As there exists no evidence that the viscosity actually diverges at any finite temperature and no real phase transition is taking place (though from a practical point of view this question is quite academic, a glass well below its glass temperature will be "frozen" essentially forever), one needs to ask himself what makes the relaxation dynamics of a glass so slow. This is a question about dynamics, not about thermodynamics (though there are also clear thermodynamic signatures of the glass "transition", which we do not discuss here). One thing is absolutely clear: we are talking here about a (strongly) out-of-equilibrium phenomenon.

To get a slightly better understanding of what actually is going on, let us consider microscopic

quantities. The van Hove correlation function is defined as

$$G(\boldsymbol{r}, t) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} \delta\left[\boldsymbol{r} - (\boldsymbol{r}_i(t) - \boldsymbol{r}_j(0))\right] \right\rangle , \tag{11.1}$$

where $< \cdot >$ is an ensemble average. Obviously the volume integral of $G(\boldsymbol{r}, t)$ just gives the number of particle N, i.e. $\int G(\boldsymbol{r}, t) d\boldsymbol{r} = N$. It is common to decompose $G(\boldsymbol{r}, t)$ into its self and distinct parts

$$G(\boldsymbol{r}, t) = G_s(\boldsymbol{r}, t) + G_d(\boldsymbol{r}, t) , \tag{11.2}$$

where the self part is given by

$$G_s(\boldsymbol{r}, t) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \delta\left[\boldsymbol{r} - (\boldsymbol{r}_i(t) - \boldsymbol{r}_i(0))\right] \right\rangle \tag{11.3}$$

and the distinct part reads

$$G_d(\boldsymbol{r}, t) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sum_{j \neq i}^{N} \delta\left[\boldsymbol{r} - (\boldsymbol{r}_i(t) - \boldsymbol{r}_j(0))\right] \right\rangle . \tag{11.4}$$

We obviously have $\int G_s(\boldsymbol{r}, t) d\boldsymbol{r} = 1$ and $\int G_d(\boldsymbol{r}, t) d\boldsymbol{r} = N - 1$. At time $t = 0$, we have

$$G(\boldsymbol{r}, 0) = \delta(\boldsymbol{r}) + \rho_N g(\boldsymbol{r}) , \tag{11.5}$$

where $\rho_N = N/V$ is the average number density and $g(\boldsymbol{r})$ is the pair distribution function (when orientations are averaged out, or for isotropic systems as we consider here, we obtain the usual radial distribution function. The Fourier transform of this function is the static structure factor). These quantities are directly measurable using scattering techniques. One striking observation about glasses is that their radial distribution function (i.e. the probability to find a particle a distance r away from a given particle at the origin) is nearly identical to that of an equilibrium liquid at a higher temperature. Therefore, there seems to be no *obvious* static signature (i.e. at the level of the radial distribution function) for the dramatic slowing down of the internal dynamics of a glass.

We should look at dynamic quantities. Let us define the intermediate scattering function (which again can be decomposed into its self and distinct parts) as the spatial Fourier transform of $G(\boldsymbol{r}, t)$

$$F(\boldsymbol{k}, t) = \int G(\boldsymbol{r}, t) e^{-i\boldsymbol{k} \cdot \boldsymbol{r}} d\boldsymbol{r} . \tag{11.6}$$

For the self part of the intermediate scattering function (ISF) we obtain

$$F_s(\boldsymbol{k}, t) = \frac{1}{N} \left\langle \sum_i e^{-i\boldsymbol{k} \cdot [\boldsymbol{r}_i(t) - \boldsymbol{r}_i(0)]} \right\rangle \equiv \langle \Phi_s(\boldsymbol{k}, t) \rangle . \tag{11.7}$$

How does this function look like? For an equilibrium liquid it simply decays exponentially with a characteristic molecular timescale (k is usually chosen to correspond to the first peak in the radial distribution function, but this is not important here). When the glass transition temperature is approached something dramatic happens. The self intermediate scattering function exhibits two-step relaxation dynamics. First, over a relatively short timescale, it drops to a value somewhat smaller than unity. Then it remains "stuck" at this level for a long time and finally it drops to zero. The final relaxation is non-exponential, but rather follows a "stretched exponential" behavior

$$F_s(\boldsymbol{k}, t) \sim e^{-(t/\tau)^\beta} \; , \tag{11.8}$$

with a stretching exponent $\beta < 1$. The characteristic relaxation time, defined as the time it takes $F_s(\boldsymbol{k}, t)$ to reach $1/e$, is denoted by τ_α. It is this timescale, the so-called α relaxation time, that grows dramatically near the glass temperature. In fact, as the main relaxation time, it is proportional to the viscosity

$$\eta \sim \tau_\alpha \; . \tag{11.9}$$

Note, however, that the stretched exponential behavior in fact implies a distribution of timescales (which is only peaked at τ_α). We can also ask what is the manifestation of this slowing down of relaxation times at the level of single particles. For that we can focus on the mean-squared-displacement $\langle r^2(t) \rangle$ and plot $\log \langle r^2(t) \rangle$ vs. $\log t$. For an equilibrium liquid the picture is clear. The behavior is ballistic (i.e. a straight line of slope 2 in the log-log plot) below a typical vibration timescale and diffusive (i.e. a straight line of slope 1 in the log-log plot) above it. Near the glass transition the curve develops a long plateau before it crosses over to a diffusive behavior. The typical timescale in which the plateau ends is again τ_α. The physical picture is that the particles are "frozen/locked" within cages formed by their neighbors and only once the cage opens up by some very low probability cooperative fluctuation of several particles, it can diffuse away. It is this cooperative motion that is believed to be at the heart of the dynamic slowing down near the glass temperature, though nobody knows how to calculate the relaxation time from first principles. These dynamics are also markedly different from an ordinary fluid in which thermal fluctuations and stress relaxation events are distributed rather homogeneously in space and occur on similar time scales. A glass is a disordered state of matter in which the thermal vibration timescales are well separated from stress relaxation timescales. This suggests a picture in which the vibrational degrees of freedom of a glass are quickly equilibrated with the heat bath, but the structural degrees of freedom are out-of-equilibrium with the bath. Obviously a major theoretical hurdle

in calculating the relaxation time is that we do not know how to handle the intrinsic structural disorder of a glass.

For an equilibrium liquid a Gaussian approximation is valid and the self-ISF can be written as

$$F_s(\boldsymbol{k}, t) \simeq \exp\left[-\frac{k^2 \langle r^2(t) \rangle}{6}\right] \ . \tag{11.10}$$

Since the diffusion coefficient is

$$D = \lim_{t \to \infty} \frac{\langle r^2(t) \rangle}{6t} \ , \tag{11.11}$$

we obtain

$$F_s(\boldsymbol{k}, t) \sim \exp\left[-Dk^2 t\right] \ . \tag{11.12}$$

As we discussed above, this is indeed the case for equilibrium liquids. The breakdown of this behavior as the glass temperature is approached, tells us that the statistics become non-Gaussian.

Vibrational anomalies and Stokes-Einstein relation violation

The disordered nature of the glassy state has some dramatic implications for vibrational excitations. In crystalline solids, the low frequency vibrational modes are extended (long wavelength) phonons, whose density of states scales as $D_{\mathrm{D}}(\omega) \sim \omega^{d-1}$ (d is the dimension), following Debye's theory (hence the subscript). Glasses of course feature low frequency phonons as well, which is just a manifestation of global continuous symmetries (the Goldstone theorem). However, they feature also other low frequency vibrations, which do not exist in their crystalline counterparts. Here we highlight major properties of these vibrational anomalies:

- *Quasi-localized glassy modes* — Very recently it has been established that the low frequency end of the vibrational spectrum of glasses features quasi-localized (non-phononic) vibrational modes in addition to low frequency phonons. These modes feature a localization length (of a few atomic sizes) and a power-law decay. Moreover, they follow a universal gapless density of states $D_{\mathrm{G}}(\omega) \sim \omega^4$.

- *The Boson peak* — At somewhat higher frequencies (typically corresponding to the terahertz range in experiments) other non-phononic vibrational excitations exist. These generically give rise to the so-called Boson peak (the name has nothing to do with the physics of Bosons) that manifests itself by plotting $D(\omega)/\omega^{d-1}$, which exhibits a peak ($D(\omega)$ is the total/measured vibrational density of states).

These vibrational anomalies are intimately related to some universal low temperature anomalies in glasses (e.g. in the thermodynamic and transport properties), which are not discussed here.

Another implication of the glass transition is related to the Stokes-Einstein relation, $\eta D \sim k_B T$, which was mentioned in our discussion of Newtonian fluids. In the glassy state, near T_g, this relation between diffusivity and viscosity is violated by a factor that can reach $10^2 - 10^3$. That is, while the diffusivity D decreases with decreasing T, it does so less dramatically than the increase in the viscosity η.

Dynamic heterogeneity and aging

It is clear from the above discussion that glassy dynamics is highly heterogeneous. In search for statistical measures of cooperativity/heterogeneity, people started looking at higher order correlation functions. One popular object is the four-point density correlation function defined as

$$C_4(\boldsymbol{r}, t) = \langle \rho(0,0)\rho(0,t)\rho(\boldsymbol{r},0)\rho(\boldsymbol{r},t) \rangle - \langle \rho(0,0)\rho(0,t) \rangle \langle \rho(\boldsymbol{r},0)\rho(\boldsymbol{r},t) \rangle \ . \tag{11.13}$$

It quantifies the spatial (different particles separated by $\boldsymbol{r}$) correlation between correlated motion in time (single particle). The hope here is to be able to extract a growing correlation length from such a correlation function. In many cases it is not easy to evaluate this correlation function and hence its spatial integral is used instead

$$\chi_4(t) = \int C_4(\boldsymbol{r}, t) d\boldsymbol{r} \ . \tag{11.14}$$

χ_4 is known as the "dynamic susceptibility" and the spatiotemporal correlated motion is termed "dynamic heterogeneity". χ_4 is regarded as a dynamical order parameter, which is also peaked at τ_α and can be used to define a cooperativity lengthscale.

We mentioned above that glasses are intrinsically out-of-equilibrium. This means, for example, that all of the standard powerful tools and results of equilibrium statistical thermodynamics (e.g. fluctuation-dissipation relations, equipartition etc.) are not valid. Another fundamental aspect of this is the phenomenon of aging. Glasses near their glass temperature spontaneously relax towards equilibrium (albeit very slowly). That means that even in the absence of external forces physical quantities (e.g. energy, volume etc.) change over time. Time translational invariance (TTI) is broken in the glassy state, i.e. it is a non-ergodic state. Following the timescales separation discussed before, it is clear that the structural degrees of freedom are those that age (they undergo structural relaxation), while the vibrational ones are equilibrated with the bath. In a

schematic manner, we may say that a glass is non-Arrhenius, non-exponential and non-ergodic.

Non-affine deformation and the elasticity of amorphous materials

One may naively think that elasticity of amorphous system is rather simple. Eventually, how complicated a generalization of a linear Hookean spring can be? The answer is that structural disorder may make even elasticity rather non-trivial. To get a feeling of that, we need to introduce the notion of non-affine deformation. Suppose we apply simple shear deformation to a solid. In a perfect crystal, the deformation of any atom is the same as the macroscopically imposed deformation. All particles respond similarly. We call this affine response. This cannot happen in a disordered (amorphous) solid. In this case, not all particles can reach local mechanical equilibrium by following the macroscopic deformation. They have to move in different directions and over different distances to conform with their local environment. The elastic response is heterogenous. We say that the deformation contains a non-affine component, i.e. part of the local deformation in the system is not the same as the macroscopically imposed one. What are the consequences of this non-affine deformation to elasticity? The non-affine deformation makes the system softer as compared to its crystalline counterpart of the same composition. The shear modulus (the bulk modulus is rather insensitive to such physical effects) can be written as

$$\mu = \mu_B - \mu_{na} \ , \tag{11.15}$$

where μ_B is the affine contribution (the one of a perfect crystal, "B" stands for "Born") and μ_{na} is associated with the non-affine deformation. μ_{na} is typically 30% of μ_B, which makes amorphous solids about 30% softer than their crystalline counterparts. Put in another way, for a given applied shear stress τ, an amorphous solid stores more elastic energy $\sim \tau^2/\mu$ than its crystalline counterpart (of the same composition). The non-affine motions provide the amorphous system with additional degrees of freedom for storing energy.

Visco-elasticity of amorphous materials

We mentioned above that glassy dynamics are characterized by a broad spectrum of relaxation times. A direct experimental evidence for that is obtained through linear mechanical spectroscopy. In particular, the loss modulus $G''(\omega)$ (defined in Eq. (9.39)) spans many orders of magnitude, i.e. it is much broader than $G''(\omega)$ for the Maxwell model which drops off linearly from its peak.

In a glass, $G''(\omega)$ is peaked at $\omega_\alpha \sim 1/\tau_\alpha$ but decays much slower away from the peak.

Effective temperatures emerging from non-equilibrium fluctuation-dissipation relations

Let us consider another intriguing feature of glassy systems. For that, we need to recall the fluctuation-dissipation theorem of equilibrium statistical physics. Consider two physical observables, say A and B, and define their two-point mutual correlation function as

$$C(t) = <A(t)B(t)> - <A(0)><B(0)> \ . \tag{11.16}$$

Introduce then a small perturbation h_B (an external field), which drives the systems gently out-of-equilibrium and which is thermodynamically conjugated to B. That is, $h_B B$ is a time-dependent perturbation to the original time-independent Hamiltonian of the system). The susceptibility $\chi(t)$ quantifies the response of the observable A to this perturbation

$$\chi(t) = \frac{<A(t) - A(0)>}{h_B} \ . \tag{11.17}$$

Note that of course one is allowed to choose $A = B$. Finally, the fluctuation-dissipation relation takes the form

$$\chi(t) = \frac{1}{k_B T} \left[C(0) - C(t) \right] \ . \tag{11.18}$$

This is one of the central features of systems at thermal equilibrium. What happens in glassy systems, either during aging or when they are persistently driven externally (the latter will be discussed soon in the context of plasticity)? Well, as these are out of equilibrium systems, we expect the equilibrium fluctuation-dissipation relation to break down. Is the breakdown interesting and insightful?

At short times, when the particles vibrate within the cages formed by their neighbours, the system is just an equilibrium system at the bath temperature T. Hence we expect the equilibrium fluctuation-dissipation relation to remain valid. This means that the vibrational degrees of freedom of a glassy material are in equilibrium at T. At longer time, where the non-equilibrium nature of the configurational degrees of freedom is crucial, we expect the relation to break down. In the last 20 years or so people studied this breakdown, both on the computer and in the lab, and discovered something remarkable: in many cases, the longer times relation between $\chi(t)$ and $C(t)$ is not some arbitrary function, but rather it remains *linear* with a slope *different* from $-1/T$ (the absolute value of the slope is generically smaller than $-1/T$). These observations have driven

people to propose that the configurational degrees of freedom of glasses are in quasi-equilibrium at an effective temperature $T_{eff} > T$ determined from the long times slope of the non-equilibrium fluctuation-dissipation relation. These ideas have triggered a lot of interest and subsequent extensive work, see the following review paper: "The effective temperature", Journal of Physics A: Mathematical and Theoretical **44**, 483001 (2011).

The issues briefly raised above, including the strongly nonlinear dissipative (plastic) response, are hot topics in the condensed-matter, statistical and materials physics communities.

XII.   THE FIELD THEORY OF PLASTICITY

Up to now we considered linear viscous deformation as a dissipative process in solids. However, the vast majority of the solids we encounter around us do not exhibit viscous flow at small applied stresses on reasonable timescales. They are elastic solids. Our focus in the rest of the course will be on what happens when such an elastic solid is subjected to large enough driving forces (we will have to quantify what we mean by large here). Again, our everyday experience already gives us a hint to what can happen. Take a metal spoon and start bending it. If the force you apply is small, the spoon bends and then recovers its original shape when you remove the force. However, if you bend it hard enough and then remove the force, the spoon will not return to its original shape. It would be permanently deformed. The material remains is a new "equilibrium" configuration that carries memory of the previous irreversible deformation. We call this phenomenon "plastic deformation". Suppose now your spoon is made of wood and you repeat your bending experiment. What would happen then? For small applied forces, the spoon will respond elastically, in much the same way as the metal spoon. However, when you bend it hard enough, it will simply break into two pieces. We call this phenomenon "fracture". In this case, the spoon also finds a new "equilibrium" configuration that carries (some, but less?) memory of the previous deformation. Intuitively, we feel that the irreversibility in the two cases is somewhat different. In the metal case, we might bend the spoon backwards to its original shape, while in the piece of wood case, the irreversibility appears stronger. The phenomena of plasticity and fracture will be discussed in the remaining of the course. These are strongly nonlinear and dissipative phenomena that are both fascinating, and of prime scientific and technological importance.

We start by looking at plasticity. Let us first consider experimental observations. Suppose one takes a metal sample and slowly increases the stress applied to it. What would the response look like? There will be an initial linear elastic response followed by a nonlinear behavior. Up to now we cannot tell whether the response is nonlinear elastic or something else. To distinguish between these possibilities, we need to unload the system, i.e. to remove the applied stress. If the response was nonlinear elastic, we would follow the loading path backwards, recovering the original state. This is not what happens for a metal. In this case, the strain will go down linearly, roughly with the same modulus of the linear elastic loading curve, hitting the zero stress at a *non-zero* strain. The system is permanently deformed and the residual strain is called plastic strain.

A.   The concept of yield stress and perfect plasticity

This physical response entails the introduction of a new concept that has to do with the critical conditions beyond which the behavior is no longer elastic (reversible), but rather plastic (irreversible). The concept we need is that of a "yield stress". It is a new stress scale in the system, in addition to elastic constants that are also of stress dimension, which tells us at what typical stress a solid starts to flow/deform plastically. In an idealized scenario, a solid behaves in an elastic-perfect plastic manner: it responds linear elastically for stresses below the yield stress σ_y and flows indefinitely at the yield stress. In this ideal case the stress cannot overshoot σ_y as plastic deformation instantaneously relaxes it back to σ_y. Plastic deformation is intrinsically related to stress relaxation processes. Mathematically, this ideal elastic-perfect plastic behavior can be captured by the following constitutive law

$$
\begin{aligned}
\sigma = E\epsilon \quad &\text{for} \quad \epsilon < \frac{\sigma_y}{E} \\
\sigma = \sigma_y \quad &\text{for} \quad \epsilon \geq \frac{\sigma_y}{E} \ .
\end{aligned}
\tag{12.1}
$$

Above yielding, the evolution is non-elastic and the power $\sigma_y \dot{\epsilon}$ is partially transformed into heat and partially locked in dynamically generated material structures, as previously discussed in the context of thermodynamics with internal variables.

The introduction of an yield stress might appear rather innocent at first sight, but it has profound consequences that make plasticity theory strongly nonlinear and highly nontrivial to study. Before we work out a few examples in order to highlight some new features, let us first generalize the ideal elastic-perfect plastic law above to situations where the stress state is three-dimensional. The basic idea is that a yield stress in the one-dimensional case discussed above transforms into a yield surface in the space of the components of the stress tensor. This surface defines an elastic domain. Inside the elastic domain, the material response is elastic. On the surface, the response is plastic. To express this mathematically, we first make the further assumption (which is experimentally supported for metals and whose microscopic origin will be discussed later) that plastic flow is largely insensitive to hydrostatic stresses, only to deviatoric (shear) ones. That is to say, we would like to express the yielding criterion in a way that is independent of $\operatorname{tr}\boldsymbol{\sigma}$. Therefore, we would like to use the deviatoric stress tensor $\boldsymbol{s} = \boldsymbol{\sigma} - \frac{1}{3}\operatorname{tr}(\boldsymbol{\sigma})\boldsymbol{I}$ as the basic object. The two simplest and rather widely used yield criteria (they are also supported experimentally to some degree) are due to von Mises and Tresca. In the von Mises criterion (1913) (the criterion was formulated by Maxwell in 1865, discussed by Huber in his 1904 work, but is usually attributed to

von Mises) one assumes that the second invariant of s, $J_2 = \frac{1}{2}s : s$, reaches a threshold value at yielding

$$\sqrt{J_2} = \sigma_y \; . \tag{12.2}$$

Note that J_2 can be expressed in terms of the principal stresses as

$$J_2 = \frac{(\sigma_1 - \sigma_2)^2 + (\sigma_3 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2}{6} \; . \tag{12.3}$$

While the von Mises criterion is based on energetic considerations, the Tresca criterion (1864) is based directly on stresses. It states that yielding takes place when the maximal shear stress along any possible orientation reaches a threshold, that is

$$\frac{1}{2}\max(|\sigma_i - \sigma_j|_{i \neq j}) = \sigma_y \; . \tag{12.4}$$

Note that σ_y here and in the von Mises criterion is not necessarily the same (both just express the idea that a threshold exists) and that when two components of the stress tensor are equal, the von Mises and Tresca criteria are essentially identical (we schematically denote the yield stress by σ_y, though a more appropriate notation would be s_y or τ_y).

B. The theoretical and practical shear strength (yield stress) — dislocations needed

Up to now we treated the yield stress σ_y as a material parameter, but we did not say anything about its magnitude. Of special interest is the relation between the yield stress and the other stress scale in a solid, the elastic modulus. In order to get a physical intuition about the yield stress, let us consider an infinite cubic lattice with a lattice constant d. It is clear that translating the lattice over a distance d brings the system back to the same configuration. It is also conceivable that a displacement smaller than $d/2$ would be reversible and a displacement larger than $d/2$ would make the configuration unstable, i.e. induce an increment of irreversible deformation. The stress that is needed to bring the system to the unstable state is the yield stress (or the shear strength). A mathematical representation of the physical situation described above is given by

$$\tau = \tau_{max} \sin\left(\frac{2\pi x}{d}\right) \; , \tag{12.5}$$

where τ is the shear stress (this dates back to Frenkel, 1926). While the sine function may not be accurate, it possesses the required properties and should provide us with rough estimates. In order to estimate τ_{max}, we note that to linear approximation we have

$$\tau \simeq \tau_{max}\frac{2\pi x}{d} \; . \tag{12.6}$$

However, linear elasticity tells us that $\tau = \mu\gamma$, where $\gamma = x/d$, and therefore

$$\tau_{max} = \frac{\mu}{2\pi} \; . \tag{12.7}$$

More sophisticated estimates for the theoretical shear strength reach somewhat smaller values, but still of the order of $10^{-1}\mu$. What do experiments tell us? Well, measured values for metals are in the range of $10^{-5}\mu - 10^{-3}\mu$, which are orders of magnitude smaller than the theoretical estimates. What went wrong? Why solids are so much weaker than their theoretical limit? The answer is that solids do NOT flow plastically by simultaneously shifting complete atomic planes. Instead, they flow by the propagation of lattice defects known as dislocations. We already encountered these objects in our discussion of linear elasticity. There (cf. Eq. (5.45) and the discussion around it), our concern was the elastic consequences of the existence of a topological defect which we defined at the continuum level as

$$\oint d\boldsymbol{u} = \boldsymbol{b} \; , \tag{12.8}$$

where $\boldsymbol{b}$ is the Burgers vector. Our focus here would be on the formation and propagation of dislocations. For that aim, we need to adopt a more microscopic perspective. Think first of a perfect square lattice in 2d and make a close rectangular path ("circuit") around some point in the lattice. Insert then an additional line of atoms above this point. This can be physically achieved by pushing atoms above some line a distance b, of the order of a lattice distance, without moving the atoms below the line. The resulting defect is called an edge dislocation and it is characterized by a Burgers vector $\boldsymbol{b}$ (there are other types of dislocations, such as screw dislocations discussed earlier, but the basic idea is the same). The latter can be obtained by realizing that the original rectangular path ("circuit") around the core of the dislocation fails to close upon itself. The vector that is needed to close the circuit is $\boldsymbol{b}$. When such a defect moves in a solid it carries with is a "quantum" of plastic deformation. For example, when it crosses a crystal from one side to another, it leaves an atomic step of size $|\boldsymbol{b}|$ on the boundary. Why does such motion require significantly smaller stress than the ideal strength? The crucial point is the elastic field generated by such a defect, which has already shown to take the form

$$\sigma \sim \frac{\mu\,|\boldsymbol{b}|}{r} \; . \tag{12.9}$$

Therefore, the stress near the dislocation core is already very intense (in the absence of an external stress) and only a relatively small external stress should be added in order to push it into motion. This basic understanding already gives us a qualitative idea about how to resolve the above puzzle.

In fact, the external stress needed to move an isolated dislocation within a perfect crystal can be estimated using the dislocation stress field and the simple interatomic stress of Eq. (12.5), assuming a continuous distribution of irreversible slip (i.e. not quantized by the Burgers vector). This model results in an integro-differential equation which was solved by Peierls (Proc. Phys. Sot. **52**, 34 (1940)) and Nabarro (Proc. Phys. Sot. **59**, 256 (1947)), yielding the Peierls-Nabarro stress which we only quote here (details will appear in the tutorial session)

$$\tau_{PN} = \frac{2\mu}{1-\nu} \exp\left[-\frac{2\pi h}{d(1-\nu)}\right] , \tag{12.10}$$

where h is the distance between adjacent atomic planes (which does not necessarily equal d). For reasonable numbers, one obtains $\tau_{PN} \sim 10^{-5}\mu$, which is consistent with the yield stress of pure single crystals. A scientifically and historically interesting paper was written by Nabarro on the occasion of "Fifty-year study of the Peierls-Nabarro stress" (Materials Science and Engineering **A234-236**, 67 (1997)). Note also that this microscopic picture of plastic flow in crystalline and polycrystalline solids immediately implies a very weak dependence on compressive stresses. In situations where there are many dislocations that interact and may hamper the motion of one another, the Peierls-Nabarro stress may not be the most important factor controlling the strength of crystalline and polycrystalline.

We finally note that dislocations are intrinsically non-equilibrium objects: the probability of finding a dislocation at equilibrium at temperatures below the melting temperature is unrealistically small. Dislocations are formed only as defects during the crystallization process and more importantly during the deformation process itself. One such dynamics formation mechanism is the Frank-Read source, which will be briefly presented in class. Dislocations mechanics and statistical mechanics constitute a fascinating and important branch of physics. Unfortunately, we will not be able to devote more time to it in the present framework. Hence, we continue to adopt a continuum approach in which the yield stress is a material parameter and bear in mind that in elasto-plastic problem there exist a small parameter of the form $\sigma_y/E \ll 1$ (or $\tau_y/\mu \ll 1$).

A historical note is in place. The concept of a dislocation in a solid was developed mathematically by Volterra in 1907. However, the fundamental relation between dislocations motion and plastic deformation in solids was not understood until 1934, when Orowan (Z. Phys. **89**, 634 (1934)), Polanyi (Z. Phys. **89**, 660 (1934)) and Taylor (Proc. R. Sot. A **145**, 362 (1934)) independently published almost simultaneous papers describing dislocation-mediated plasticity. The concept of a dislocation has revolutionized our understanding of many physical processes. For example, melting in 2d was not properly understood until Nelson and Halperin published

in 1979 their seminal paper entitled "Dislocation-mediated melting in two dimensions" (Physical Review B **19**, 2457 (1979)).

C. The continuum (field) theory of elaso-perfect plasticity

Let us now see how such an elasto-perfect plasticity theory actually works at the continuum level. Plasticity models usually do not allow to determine a solution by static considerations alone (we say that plasticity problems are not statically determinate), but we will focus on situations when this is possible. In general, the dynamic path that the deformation follows should be calculated in order to find a solution. From a fundamental physics point of view, plasticity is an intrinsically dynamic phenomenon and hence a statically determinate problem is by no means representative. Nevertheless, such an example can be worked out analytically and will teach us a lot.

Example: Internally pressurized spherical shell (thick-walled)

Let us consider a spherical shell of inner radius a and an outer radius b, under internal pressure of magnitude p. The thick-wall condition implies that the shell's thickness $b - a$ is not much smaller than a. Due to the symmetry of the problem, the only non-vanishing component of the displacement field is $u_r(\boldsymbol{r}) = u(r)$. We will use the following shorthand notation: $\sigma_{rr} \to \sigma_r$, $\sigma_{\theta\theta} \to \sigma_\theta$ and $\sigma_{\phi\phi} \to \sigma_\phi$ (and similarly for the components of the strain tensor). The boundary conditions are given by

$$\sigma_r(r = a) = -p \quad \text{and} \quad \sigma_r(r = b) = 0 \ . \tag{12.11}$$

Our goal is to quantitatively understand the elasto-plastic deformation of the shell. We assume small strains, even though plastic flow usually implies large strains (we want to get some insight about plasticity, keeping the mathematics as simple as possible). The strains in the problem are given by

$$\varepsilon_r = \frac{du}{dr} \quad \text{and} \quad \varepsilon_\phi = \varepsilon_\theta = \frac{u}{r} \ . \tag{12.12}$$

These kinematic relations imply the following compatibility relation

$$\varepsilon_r = \frac{d}{dr}\left(r\varepsilon_\theta\right) \ . \tag{12.13}$$

In addition, quasi-static force balance takes the form

$$\frac{d\sigma_r}{dr} + 2\frac{\sigma_r - \sigma_\theta}{r} = 0 \ . \tag{12.14}$$

As a preparatory step, we first focus on a purely linear elastic constitutive behavior, that is

$$\varepsilon_r = \frac{1}{E}\left(\sigma_r - 2\nu\sigma_\theta\right) \ , \tag{12.15}$$

$$\varepsilon_\theta = \varepsilon_\phi = \frac{1}{E}\left[(1 - \nu)\sigma_\theta - \nu\sigma_r\right] \ . \tag{12.16}$$

Substitute these constitutive equations into the kinematic relation in Eq. (12.13) to obtain (after some straightforward algebra)

$$\frac{d}{dr}\left[(1 - \nu)\sigma_\theta - \nu\sigma_r\right] = \frac{(1 + \nu)(\sigma_r - \sigma_\theta)}{r} \ . \tag{12.17}$$

The force balance in Eq. (12.14) implies $2(\sigma_r - \sigma_\theta) = -rd\sigma_r/dr$, which can be substituted in the above equation to yield

$$\frac{d}{dr}\,\mathrm{tr}\,\boldsymbol{\sigma} = \frac{d}{dr}\left[2\sigma_\theta + \sigma_r\right] = 0 \ . \tag{12.18}$$

The last result implies that $2d\sigma_\theta/dr = -d\sigma_r/dr$, which leads to

$$\frac{2}{3}\frac{d(\sigma_\theta - \sigma_r)}{dr} = -\frac{d\sigma_r}{dr} \ . \tag{12.19}$$

Substituting this in the force balance in Eq. (12.14), we obtain

$$\frac{d(\sigma_\theta - \sigma_r)}{dr} + 3\frac{(\sigma_\theta - \sigma_r)}{r} = 0 \ . \tag{12.20}$$

Eqs. (12.18) and (12.20) are two first order linear differential equations that can be readily solved to yield

$$2\sigma_\theta + \sigma_r = 3A \quad \text{and} \quad \sigma_\theta - \sigma_r = \frac{3B}{r^3} \ , \tag{12.21}$$

where A and B are constants of integration. We can then obtain $\sigma_r(r) = A - 2Br^{-3}$ and determine A and B from the boundary conditions in Eqs. (12.11), leading to

$$A = \frac{2B}{b^3} \quad \text{and} \quad B = \frac{p}{2(a^{-3} - b^{-3})} \ . \tag{12.22}$$

Therefore the linear elastic solution inside the shell $(a < r < b)$ reads

$$\sigma_r(r) = -\frac{p}{b^3/a^3 - 1}\left(\frac{b^3}{r^3} - 1\right) \ , \tag{12.23}$$

$$\sigma_\theta(r) = \frac{p}{b^3/a^3 - 1}\left(\frac{b^3}{2r^3} + 1\right) \ . \tag{12.24}$$

Since perfect plasticity is defined as the boundary of the elasticity domain, we can immediately gain insight about the onset of plastic deformation using the purely elastic solution. What is then the elastic limit?

To answer this question we need to adopt a yield criterion. Since the stress state in the shell is such that $\sigma_\theta = \sigma_\phi$, the von Mises and Tresca criteria are the same, leading to

$$\sigma_\theta - \sigma_r = \sigma_y . \tag{12.25}$$

We can use the elastic solution derived above to evaluate $\sigma_\theta - \sigma_r$, giving

$$\sigma_\theta - \sigma_r = \frac{p}{b^3/a^3 - 1} \frac{3b^3}{2r^3} . \tag{12.26}$$

Since $\sigma_\theta - \sigma_r$ is a monotonically decreasing function of r, it attains its maximum at the inner edge of the shell, $r = a$. Therefore, the yield criterion in Eq. (12.25) is satisfied first when $p = p_E$ with

$$p_E = \frac{2\sigma_y}{3} \left(1 - \frac{a^3}{b^3} \right) . \tag{12.27}$$

This means that for $p > p_E$, the solution is no longer elastic, but rather elasto-plastic. We will now explore such situations.

Since the yield criterion we use is sharp, when $p > p_E$ we expect to find a sharp boundary (in real space) between plastic and elastic domains. Let us denote the radius of this elastic-plastic boundary by c, where $a < c < b$. Since we know that the yield criterion is first met at $r = a$, it is clear that the plastic domain spans $a < r < c$ and the elastic one spans $c < r < b$. Let us focus first on the latter. Suppose now that the plastic solution, which we do not know at present, induces a pressure p_c at $r = c$. Therefore, the solution in Eqs. (12.23)-(12.24) is valid when we replace p with p_c and a with c, leading to

$$\sigma_r(r) = -\frac{p_c}{b^3/c^3 - 1} \left(\frac{b^3}{r^3} - 1 \right) , \tag{12.28}$$

$$\sigma_\theta(r) = \frac{p_c}{b^3/c^3 - 1} \left(\frac{b^3}{2r^3} + 1 \right) , \tag{12.29}$$

for $c < r < b$. Note that c and p_c are still unknown here. These two unknowns can be interrelated without knowing the solution in the plastic domain because we know that $\sigma_\theta(c) - \sigma_r(c) = \sigma_y$. Using this condition we obtain

$$p_c = \frac{2\sigma_y}{3} \left(1 - \frac{c^3}{b^3} \right) , \tag{12.30}$$

which leads to

$$\sigma_r(r) = -\frac{2\sigma_y}{3} \left(\frac{c^3}{r^3} - \frac{c^3}{b^3} \right) , \tag{12.31}$$

$$\sigma_\theta(r) = \frac{2\sigma_y}{3} \left(\frac{c^3}{2r^3} + \frac{c^3}{b^3} \right) , \tag{12.32}$$

which is again valid for $c < r < b$. c cannot be calculated without knowing the solution in the plastic domain.

The plastic domain is characterized by a constitutive law which is different from the one in the elastic domain. For our ideal elastic-perfect plastic relation, the constitutive relation for $a < r < c$ reads

$$\sigma_\theta(r) - \sigma_r(r) = \sigma_y , \tag{12.33}$$

i.e. the yield condition is satisfied everywhere in this region instead of the linear elastic constitutive relation of Eqs. (12.15)-(12.16). Note the qualitative change in the character of the constitutive law; while the elastic constitutive law is expressed as a relation between stresses and strains, the plastic one is expressed in terms of stresses alone. Using the constitutive law inside the force balance Eq. (12.14), we obtain

$$\frac{d\sigma_r}{dr} = \frac{2\sigma_y}{r} , \tag{12.34}$$

which can be readily integrated from r to c to yield

$$\sigma_r(r) = \sigma_r(c) - 2\sigma_y \log\left(\frac{c}{r}\right) . \tag{12.35}$$

σ_r should be continuous at $r = c$ (though its derivative is not), so using Eq. (12.31) we obtain

$$\sigma_r(r) = -\frac{2\sigma_y}{3}\left[1 - \frac{c^3}{b^3} + 3\log\left(\frac{c}{r}\right)\right] . \tag{12.36}$$

$\sigma_\theta(r)$ simply satisfies

$$\sigma_\theta(r) = \sigma_r(r) + \sigma_y . \tag{12.37}$$

Note that the continuity of σ_θ at $r = c$ is automatically satisfied and does not provide with an additional constraint. The last remaining thing we need before the complete solution is obtained is to determined c. For that aim, we use the boundary condition $\sigma_r(a) = -p$, which directly leads to

$$p = \frac{2\sigma_y}{3}\left[1 - \frac{c^3}{b^3} + 3\log\left(\frac{c}{a}\right)\right] . \tag{12.38}$$

This equation should be solved numerically for c. Note that the different constitutive laws in the elastic and plastic domains give rise to different behaviors of the stress; in the elastic domain the stress varies spatially as a power-law, while in the plastic domain it varies logarithmically.

Finally, we may ask ourselves what is the "Ultimate pressure" p_U, i.e. the pressure for which the whole shell becomes plastic. This is simply determined by the condition $c = b$, which leads to

$$p_U = 2\sigma_y \log\left(\frac{b}{a}\right) . \tag{12.39}$$

Therefore, for $p \leq p_E$ the shell is fully elastic, for $p_E < p < p_U$ the shell is elasto-plastic and for $p = p_U$ it is fully plastic.

Once the complete stress distribution is known, one can also calculate the displacement $u(r)$. Within the elastic region, $c < r < b$, one simply uses

$$u(r) = \varepsilon_\theta \, r = \frac{r}{E} \left[(1 - \nu)\sigma_\theta(r) - \nu\sigma_r(r) \right] \ , \tag{12.40}$$

where $\sigma_r(r)$ and $\sigma_\theta(r)$ of Eqs. (12.31)-(12.32) are used, with c which is determined from Eq. (12.38). To calculate $u(r)$ in the plastic region, we need to bear in mind that stresses always emerge due to elastic strain. Moreover, plasticity is quite generically deviatoric in nature and the volumetric strain is purely elastic. Consequently, we can use the linear elastic relation $\mathrm{tr}\,\boldsymbol{\varepsilon} \propto \mathrm{tr}\,\boldsymbol{\sigma}$ to obtain

$$\frac{du}{dr} + 2\frac{u}{r} = \frac{1}{r^2}\frac{d\,(r^2\,u)}{dr} = \frac{1 - 2\nu}{E}(\sigma_r + 2\sigma_\theta) \ , \tag{12.41}$$

which can be readily integrated using Eqs. (12.36)-(12.37) and demanding continuity of the displacement at $r = c$. We stress again that these explicit relations between stresses and displacements are not generic and are rather specific to this example.

Plastic deformation may lead to various interesting and surprising physical effects. We already mentioned that plastic deformation implies residual plastic strains. Actually, when the deformation is spatially inhomogeneous, residual stresses remain locked in the solid as well. These residual stresses may, and generally do, affect the subsequent response to additional loading cycles. Sometimes this may strengthen the material, leading to a phenomenon known as *shakedown* — a situation in which no further plastic deformation occurs after one or a few deformation cycles — that is, all subsequent unloading-reloading cycles are elastic. Another important phenomenon is that of unlimited plastic flow (plastic collapse), in which a solid deforms continuously at a fixed applied stress. We will encounter some of these phenomena below.

Example: Plastic cavitation

Before we continue our discussion of the physics of plastic deformation, let us consider another example, still in the framework of the elastic-perfect plastic model. Earlier in the course, we considered the problem of elastic cavitation in soft solids. Can we analyze a similar problem for hard solids?

The answer is definitely yes, such an analogous phenomenon exists for hard solids, though the physical processes is different; while for soft solids elastic deformation can be very large and lead

to cavitation, hard solids show a limited range of elastic response and the origin of cavitation is plastic deformation.

We follow the kinematic analysis leading to Eq. (7.58), which is reproduced here

$$\lambda_r = \left(1 + \frac{L^3 - \ell^3}{r^3}\right)^{2/3} , \tag{12.42}$$

where λ_r is the radial stretch, L is the radius of the undeformed cavity and ℓ is the radius of the deformed one. The logarithmic strain ϵ_r reads

$$\epsilon_r = \log \lambda_r = \frac{2}{3} \log\left(1 + \frac{L^3 - \ell^3}{r^3}\right) . \tag{12.43}$$

Note that we use the logarithmic strain because it is thermodynamically-conjugated to the Cauchy stress that we use next. The force balance equation in terms of the Cauchy stress is given in Eq. (12.14) and the boundary conditions are

$$\sigma_r(r = \ell) = 0 \quad \text{and} \quad \sigma_r(r \to \infty) = \sigma^\infty . \tag{12.44}$$

Since symmetry implies $\sigma_\theta = \sigma_\phi$ and we assume incompressibility, the stress state is essentially uniaxial and we can write down a general constitutive law as

$$\sigma_r - \sigma_\theta = \sigma_y f(\epsilon_r) . \tag{12.45}$$

We then have

$$\int_\ell^\infty d\sigma_r = -2\sigma_y \int_\ell^\infty \frac{f(\epsilon_r) dr}{r} = -2\sigma_y \int_\ell^\infty f\left[\frac{2}{3} \log\left(1 + \frac{(L/\ell)^3 - 1}{(r/\ell)^3}\right)\right] \frac{d(r/\ell)}{(r/\ell)}$$

$$\implies \sigma^\infty = -2\sigma_y \int_1^\infty f\left[\frac{2}{3} \log\left(1 + \frac{(L/\ell)^3 - 1}{x^3}\right)\right] \frac{dx}{x} . \tag{12.46}$$

The cavitation threshold σ_c is defined as the stress needed to grow the cavity indefinitely, i.e. $\ell \gg L$. This leads to

$$\sigma_c = \lim_{\ell \to \infty} \sigma^\infty = -2\sigma_y \int_1^\infty f\left[\frac{2}{3} \log\left(1 - x^{-3}\right)\right] x^{-1} dx . \tag{12.47}$$

The constitutive law $(\sigma_r - \sigma_\theta)/\sigma_y = f(\epsilon_r)$ we adopt is that of Eq. (12.1), which we interpret here as pertaining to the logarithmic strain and also allow all quantities to be signed,

$$f(\epsilon_r) = \frac{\epsilon_r}{\epsilon_y} \quad \text{for} \quad |\epsilon_r| < \epsilon_y$$
$$f(\epsilon_r) = \text{sign}(\epsilon_r) \quad \text{for} \quad |\epsilon_r| \geq \epsilon_y , \tag{12.48}$$

where $\epsilon_y \equiv \sigma_y/E$. With this law at hand, after a few rather simple mathematical manipulations, we obtain a nice analytic result. First, we use the yield strain ϵ_y inside the argument of $f(\cdot)$ in the above integral

$$-\epsilon_y = \frac{2}{3} \log \left(1 - x_y^{-3}\right) \qquad \Longrightarrow \qquad x_y = [1 - \exp(-3\epsilon_y/2)]^{-1/3} \ . \tag{12.49}$$

This allows us to use the constitutive law in order to split the integral into its elastic and plastic contributions as

$$\frac{\sigma_c}{\sigma_y} = \underbrace{2 \int_1^{x_y} x^{-1} dx}_{\text{Plastic domain}} - \underbrace{\frac{4}{3\epsilon_y} \int_{x_y}^{\infty} \log \left(1 - x^{-3}\right) x^{-1} dx}_{\text{Elastic domain}} \ . \tag{12.50}$$

We now recall that there exists a small parameter in the problem, $\epsilon_y \ll 1$ (since for ordinary hard solids the yield stress is much smaller than the elastic modulus). Therefore, we have

$$x_y \simeq \left(\frac{2}{3\epsilon_y}\right)^{1/3} \gg 1 \quad \text{and} \quad \log\left(1 - x^{-3}\right) \simeq -x^{-3} \ . \tag{12.51}$$

This immediately yields

$$\frac{\sigma_c}{\sigma_y} \simeq 2 \log(x) \Big|_1^{\left(\frac{2}{3\epsilon_y}\right)^{1/3}} - \frac{4}{3\epsilon_y} \times \frac{x^{-3}}{3} \Big|_{\left(\frac{2}{3\epsilon_y}\right)^{1/3}}^{\infty} = \frac{2}{3} \log\left(\frac{2}{3\epsilon_y}\right) + \frac{2}{3} \ . \tag{12.52}$$

Therefore,

$$\frac{\sigma_c}{E} \simeq \frac{2\epsilon_y}{3} \left[1 + \log\left(\frac{2}{3\epsilon_y}\right)\right] \ . \tag{12.53}$$

As expected, σ_c is an increasing function of σ_y (for a fixed E), but the dependence is not trivial and could not have been guessed to begin with (note, though, that the elastic term is related to the elasticity limit presented in Eq. (12.27) in the $b/a \to \infty$ limit). This is an example of unlimited plastic flow under a fixed applied stress ("plastic collapse").

D. Beyond perfect plasticity

The elastic-perfect plastic model discussed above involves some serious simplifications. One simplification we adopted is that elasto-plastic materials behave in a perfect plastic manner, i.e. flow indefinitely at a yield stress that cannot be exceeded. This is not quite true for most of the materials. This brings us to a very important phenomenon called "strain hardening" or "work hardening", which means that the stress needed to make a solid flow plastically is increasing with the deformation beyond the initial yield stress (elastic limit) σ_y. The material becomes plastically

harder (stronger) the more it is deformed. Usually the increase of the stress with strain can be described by a power-law and hence in many cases one phenomenologically replaces Eq. (12.1) with

$$
\begin{aligned}
\sigma &= E\epsilon && \text{for} \quad \epsilon < \frac{\sigma_y}{E} \\
\sigma &= \sigma_y \left(\frac{E\epsilon}{\sigma_y}\right)^n && \text{for} \quad \epsilon \geq \frac{\sigma_y}{E} \ ,
\end{aligned}
\tag{12.54}
$$

where n is the hardening exponent (typically small). For $n = 0$ we recover the elastic-perfect plastic law. Another way to describe hardening, say in the framework on the J_2 theory of Eq. (12.2), is to stipulate that the yield stress is in fact a function of the history of the deformation, i.e.

$$
\sqrt{J_2} = f(\beta) \ ,
\tag{12.55}
$$

where β is sometimes taken to be proportional to the plastic dissipation $\int_0^t \dot{\epsilon}^{pl} : \sigma \, dt'$. In order to get a better qualitative understanding of strain hardening, we need again to consider the microscopic processes that mediate plasticity – dislocations dynamics. Qualitatively speaking, some of the dislocations that move chaotically during plastic deformation remain locked inside the material ("statistically stored dislocations") and serve as obstacles for additional flow. Understanding strain hardening from basic principles remains one of the major challenges in materials physics.

Another great simplification in the ideal elastic-perfect plastic model is the omission of all dynamical aspects of plasticity, including the relevant timescales. Plasticity is an intrinsically dynamic phenomenon. From this perspective, we would expect the theory to tell us some basic about rates (i.e. strain rates instead of strains) and the basic field to be the velocity field (instead of the displacement field). Therefore, we would like to express elastic-plastic theories in terms of the rate of deformation tensor D, which is a symmetrized version of the velocity gradient tensor L (when small deformations are of interest, D can be approximated by the total strain rate tensor $\dot{\epsilon}$). This immediately poses a very serious problem that was alluded to earlier in the course. Elasticity involves a memory of one reference state and is described by the displacement field that is defined with respect to the reference configuration. Plasticity, on the other hand, implies the continuous evolution of the configuration and is generally described by the velocity field in the deformed configuration. Elasticity seems to be more naturally described in Lagrangian coordinates, while plasticity seems to be more naturally described in Eulerian coordinates. How do we combine them together?

This is a very serious problem that goes beyond the scope of our discussion. We will only

briefly mention that one can roughly distinguish between two basic approaches to this problem. In the first of these, one decomposes the deformation gradient $\boldsymbol{F}$ (recall that $\boldsymbol{L} = \dot{\boldsymbol{F}}\boldsymbol{F}^{-1}$) into a product of a plastic part $\boldsymbol{F}^{pl}$ and an elastic one $\boldsymbol{F}^{el}$ as

$$\boldsymbol{F} = \boldsymbol{F}^{el}\boldsymbol{F}^{pl} . \tag{12.56}$$

In this multiplicative decomposition, due to Kröner (1960) and Lee (1969), the order of operation is crucial. Since the deformation gradient is defined in terms of a fixed reference configuration (recall that it describes how line elements in the reference configuration are transformed into their images in the current (deformed) configuration), $\boldsymbol{F}^{pl}$ acts on such a fixed reference configuration. It describes the evolution of the structure due to plastic deformation and transforms the reference configuration into an artificial "intermediate" configuration. Elasticity is defined with respect to this intermediate configuration and transforms it into the current (deformed) configuration. Thus, elasticity – in this framework – is defined as usual by an elastic energy functional, but with respect to an evolving configuration whose dynamics are described by the plastic deformation. This is an intrinsically Lagrangian framework in which, in some sense, plasticity is formulated in a way similar to elasticity. While this framework is not free from problems, it is very popular in formulating elasto-plasticity theories. One problem with the multiplicative decomposition is that it requires that the intermediate configuration be stress free (as always, all stresses emerge from the elastic part of the deformation). However, when the deformation is inhomogeneous (as it is usually the case) this implies that the intermediate configuration is *not* geometrically compatible (different material elements relax in a mutually incompatible way when the stress on them is relaxed).

The second conventional way to kinematically combine elasticity and plasticity is to represent elasticity in a rate form. That is, instead of defining elasticity with respect to a reference frame, we define it incrementally with respect to the current configuration. Therefore, the elastic part of the rate of deformation tensor, $\boldsymbol{D}^{el}$, is defined as the material derivative of some elastic strain

$$\boldsymbol{D}^{el} = \frac{D\boldsymbol{\epsilon}^{el}}{Dt} . \tag{12.57}$$

When an elastic constitutive relation of the form $\boldsymbol{\epsilon}^{el}(\boldsymbol{\sigma})$ is inserted, the above expression describes the time evolution of the stress $\boldsymbol{\sigma}$. The total rate of deformation tensor $\boldsymbol{D}$ is then decomposed additively as

$$\boldsymbol{D} = \boldsymbol{D}^{el} + \boldsymbol{D}^{pl} , \tag{12.58}$$

where the plasticity theory is described by $\boldsymbol{D}^{pl}$ (which by itself can depend on other variables in addition to the stress, see below). This is an intrinsically Eulerian framework in which, in some sense, elasticity is formulated in a way similar to plasticity. This formulation is also not free of problems, the major one is that it is not possible to guarantee that the rate form of elasticity will be exactly integrable, i.e. that it will lead to a path independent elastic deformation. However, one can show that for small elastic deformation (extension and rotation) both the multiplicative and the additive elasto-plastic decompositions discussed above agree with one another. We will therefore adopt the additive form and focus on simple situations where it can be written in terms of strain rates as

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^{el} + \dot{\boldsymbol{\epsilon}}^{pl} \ , \tag{12.59}$$

where $\dot{\boldsymbol{\epsilon}}^{el}$ is simply the time rate of change of Hooke's law. Plasticity is described in a rate form and contained in $\dot{\boldsymbol{\epsilon}}^{pl}$. There are many models for $\dot{\boldsymbol{\epsilon}}^{pl}$. The simplest, and probably the oldest (dating back to 1922), is due to Bingham who proposed the following (scalar) form

$$\begin{aligned} \dot{\epsilon}^{pl} &= 0 \quad \text{for} \quad \sigma < \sigma_y \\ \dot{\epsilon}^{pl} &= \frac{\sigma - \sigma_y}{\eta} \quad \text{for} \quad \sigma \geq \sigma_y \ , \end{aligned} \tag{12.60}$$

where η is a viscosity-like parameter (here we immediately see the presence of relevant plasticity timescales, which are missing altogether in the perfect plasticity model). This is the simplest way to combine the concept of a yield stress with a Newtonian-type flow. Materials described by such a model are typically termed "yield-stress fluids", which constitute an important example of complex, non-Newtonian fluids. In this context it worthwhile mentioning the Herschel-Bulkley fluids, which are described by the following stress strain-rate relation

$$\sigma = \sigma_y + \kappa \, \dot{\epsilon}^m \ , \tag{12.61}$$

which describe the flow behavior of many complex fluids/solids (clay slurries, paints, microgels, emulsions, colloidal suspensions, foams, cements, mud, polymers, organic materials and more). Note that since we do not consider here elastic deformations, we do not need to distinguish between elastic and plastic components. For $\sigma_y = 0$ and $m = 1$, we obtain a Newtonian fluid. For $\sigma_y \neq 0$ and $m = 1$, we obtain a Bingham material. More generally, the exponent m can be different from unity ("power-law fluids"). When $m > 1$, the behavior is termed "shear-thickening" while for $m < 1$, it is termed "shear-thinning". These names refer to the dependence of the nonlinear (effective) viscosity on the shearing rate

$$\eta_{eff} \equiv \frac{\partial \sigma}{\partial \dot{\epsilon}} \sim \dot{\epsilon}^{m-1} \ . \tag{12.62}$$

For $m > 1$, η_{eff} increases with the shearing rate, i.e. the fluid "thickens", while for $m < 1$, η_{eff} decreases with the shearing rate, i.e. the fluid "thins". We finally note that plasticity models whose basic object is $\dot{\epsilon}^{pl}$ are sometimes termed visco-plastic models. The "visco" part denotes the fact that these models include a timescale in them (which are absent in perfect plasticity models).

The most serious simplification of the ideal elastic-perfect plastic model, which in a deep sense includes in it the previous simplifications and which is shared by many phenomenological models of plasticity, is that it does not tell us anything about the evolution of the material's structure during deformation and how the structure affects the flow. We said several times earlier in the course that the essence of plastic (irreversible) deformation is that the configuration of the material evolves and determines the subsequent response. We also said that plastic deformation implies some "memory" of previous deformation. There are direct experimental observations that demonstrate the need to describe the evolution of the internal structure of a deforming solid. We demonstrate it here using a well-known effect, the Bauschinger effect. Consider a solid under the application of a stress that is larger than its yield stress and then unload it. The material remains deformed plastically in the absence of external stress. Ask yourself then what stress in the opposite direction would you need to apply to the material in order to recover the original shape (under stress now)? In particular, would the magnitude of this stress be equal, smaller or larger than the magnitude of the original stress? The answer is that it is smaller. Alternatively, you can apply the same magnitude of stress in the opposite direction and the response would be stronger. The material "remembers" part of its past deformation, and this should be accounted for in our theoretical modeling.

These observations and discussion clearly point to something we already know, i.e. one needs to identify coarse-grained "internal variables" that account for the material's structural evolution during plastic deformation and its effect on subsequent deformation. In the crystal plasticity problem, these are likely to include the density of dislocations and related quantities. Discussing in detail such theories goes beyond the scope of this course.

Dissipative phenomena in solid mechanics

XIII.   MATERIAL FAILURE

When solids are sufficiently strongly driven by mechanical forces, they break. The scientific field that addresses materials failure is called "Fracture Mechanics". Our goal in this part of the course is to understand the basic concepts related to the fracture of solids.

A.   Some scaling arguments

Consider a solid of cross-section A and height H. The gravitational potential energy of the solid is given by

$$U = \int g\, h\, dm = \int_0^H g\, h\, \rho A dh = \frac{\rho g A H^2}{2} \ . \tag{13.1}$$

Consider now what happens if instead of one piece of a material of height H, we have two pieces of height $H' = H/2$ (the cross-section remains the same). In this case, the total gravitational energy is given by

$$2U' = 2\frac{\rho g A}{2}\frac{H^2}{4} = \frac{U}{2} < U \ . \tag{13.2}$$

The gravitational energy *reduced* by an amount

$$\Delta U = U - 2U' = \frac{\rho g A H^2}{4} \ . \tag{13.3}$$

This is, of course, not the only energy involved. In comparing the two configurations (one vs. two pieces), we should also take into account the fact that the latter includes an additional surface (actually two). That means an *increase* in energy due to surface energy by an amount $2\gamma A$, where γ is the surface energy. Therefore the total energy of the solid can be reduced by breaking it to two identical pieces when

$$\frac{\rho g A H^2}{4} > 2\gamma A \ . \tag{13.4}$$

That means that the critical height H_c at which the solid becomes unstable scales as

$$H_c \sim \sqrt{\frac{\gamma}{\rho\, g}} \ . \tag{13.5}$$

In order to estimate H_c, we need to put in some numbers. How do we estimate the surface energy γ of ordinary solids? Surface energy has the dimensions of energy per unit area. To

estimate it we need a typical energy scale and a typical area scale. As before, we use microscopic quantities, an atomic interaction energy scale, $\sim$ 1eV, and an atomic area, $\sim 10 \times 10^{-20}\text{m}^2$ to get

$$\gamma \sim \frac{10^{-19}\,\text{J}}{10 \times 10^{-20}\,\text{m}^2} = 1\,\text{J/m}^2 \ . \tag{13.6}$$

Using $\rho \simeq 10^3 \text{kg/m}^3$ and $g \simeq 10\text{m/sec}^2$ we obtain $H_c \sim 10^{-2}\text{m}$. That is a remarkable observation. It says that essentially all solids around us are out-of-equilibrium. More accurately, they are in metastable states that can persist for extremely long times without getting to their true ground-state.

Let us now try to estimate the barrier that needs to be overcome in order to separate a solid into two pieces. For that aim, let us forget about gravitational potential energy, which is typically small compared to strain energies, and ask ourselves how much we need to stretch a solid in order to break it. Suppose we impose a uniaxial tensile strain of magnitude ϵ to a solid. What happens at the microscopic level? Let us focus on single crystals (e.g. forget about disorder, non-affine deformations etc.). In this case, the distance between atoms within the solid increases by $100 \times \epsilon$ percent. When does the interaction between two atoms drop to zero? Consider then a typical atomic interaction energy. It is clear that when the equilibrium separation is increased by a sizable fraction, say by 50%, the interaction essentially vanishes. The critical separation is somewhere in between, say at 25%. Therefore, the critical strain is roughly $\epsilon_c \simeq 0.25$. This suggests that

$$\sigma_c = E\epsilon_c \simeq \frac{E}{4} \ . \tag{13.7}$$

Note the similarity of this estimate to the ideal shear strength (shear yield stress) estimate for the plastic flow of solids. To test this prediction we again need experiments. What do laboratory experiments tell us? Well, the typical tensile strength observed in the lab is 2-3 orders of magnitude smaller than the theoretical prediction.

To understand what went wrong in the theoretical prediction, we need to better understand the dynamical processes that lead to the failure of materials. Equilibrium thermodynamics is not enough. Like in the case of plastic shear flow, where we invoked the dynamics of atomic scale defects (dislocations), also here in the context of tensile failure we need a symmetry breaking, out-of-equilibrium, dynamical process that will provide us a path to equilibrium. In this case, the objects of interest are cracks. Cracks are very interesting and important objects. In the remaining parts of the course we will try to understand their basic properties and their effect on the strength and failure of solids. Before we derive more rigorous and fundamental results, let us again start with some simple scaling arguments.

A tensile crack is defined as a material line that cannot support tensile and shear stresses, i.e. the crack faces satisfy traction-free boundary conditions $\sigma_{nn} = \sigma_{tn} = 0$ (this implies that under compressive stresses we might not be able to detect the presence of cracks). Mathematically speaking, a crack is a branch-cut that introduces a displacement discontinuity when it is crossed. Before we explore the field theoretic implications of this, we first consider a simple scaling approach. For that aim, consider an infinite solid which contains a crack of length ℓ under the application of a uniaxial stress σ (oriented perpendicularly to the crack). We will soon consider what happens when the crack propagates at a velocity v, but first focus on the case when the crack is stationary/quasi-static ($v \to 0$). Let us estimate the total energy change per unit sample thickness $\Delta \mathcal{E}$ due to the presence of a crack. In the absence of a crack, the solid is uniformly stressed with a potential strain energy density of the form

$$u_p \sim \frac{\sigma^2}{2E} \tag{13.8}$$

where E is the Young's modulus. As we said above, a crack cannot support stresses and hence strain energy is released in its surroundings. The spatial scale where it happens must be determined by ℓ, the only available scale in the problem. Therefore the change in the strain energy per unit sample thickness reads

$$\Delta \mathcal{E}_p \sim -\alpha \frac{\sigma^2 \, \ell^2}{2E} \ , \tag{13.9}$$

where α is a dimensionless number of order unity. The minus sign represents the fact that we are talking here about a reduction in the energy. It is important to note that we focuss here only on the linear elastic manifestations of the presence of the crack, a point that we will elaborate on later. As should be clear now from the above discussion, there is always a positive contribution to the energy change, coming from surface energy. This contribution is linear in ℓ and reads

$$\Delta \mathcal{E}_s \sim \gamma \ell \ . \tag{13.10}$$

In fact, we should have used here a more general concept than the surface energy – the fracture energy – to be discussed later. $\Delta \mathcal{E}$ is then expressed as

$$\Delta \mathcal{E} = \Delta \mathcal{E}_p + \Delta \mathcal{E}_s \sim -\alpha \frac{\sigma^2 \, \ell^2}{2E} + \gamma \ell \ . \tag{13.11}$$

Think now of ℓ as a thermodynamic variable and plot how $\Delta \mathcal{E}$ varies with it. At small crack lengths, the surface energy dominates the elastic energy and $\Delta \mathcal{E}$ increases with increasing ℓ. For sufficiently large cracks, the elastic energy reduction dominates and $\Delta \mathcal{E}$ decreases with increasing ℓ, implying an instability in which the crack grows indefinitely and the material undergoes

catastrophic failure. The critical crack length ℓ_c is determined from

$$\frac{\partial \mathcal{E}}{\partial \ell} = 0 \quad \Longrightarrow \quad \ell_c \sim \frac{\gamma E}{\sigma^2} \ . \tag{13.12}$$

The critical crack length decreases as the square of the applied stress. Alternatively, if ℓ is fixed – i.e. it is a frozen-in defect in the solid, which is the most common case – then the critical stress for failure σ_c reads

$$\sigma_c \sim \sqrt{\frac{\gamma E}{\ell}} \ . \tag{13.13}$$

This provides us with a deep physical insight: the strength of materials is determined by the largest defect (crack) it contains. This observation suggests a qualitative understanding of the failure of the theoretical tensile strength prediction; materials contain defects and therefore their strength is significantly reduced. We will get deeper insights about this point soon when we discuss more rigorous results. An equivalent, yet meaningful, way to combine the two last results is to write for the critical point the following relation

$$\sigma^2 \ell \sim \gamma E \ . \tag{13.14}$$

The right hand side is a combination of material parameters and the left hand side is a product of an externally controlled parameter (σ) and a parameter characterizing the defect state of the material (ℓ). This fundamental result was essentially obtained by Alan Arnold Griffith, a British engineer, in a brilliant and revolutionary series of papers in the early 1920's. The importance of Griffith's work was largely unrecognized until the 1950's. It took, then, a few more decades before this has been consolidated into a physical theory formulated within a firm mathematical framework.

Let us now consider what happens when $\ell > \ell_c$, still in the spirit of a scaling theory. When the unstable regime $\ell > \ell_c$ is approached, the crack continuously accelerates and hence emits kinetic energy into its surroundings. Therefore, a kinetic energy contribution to $\Delta \mathcal{E}$ should be taken into account. Suppose the crack propagates (at least instantaneously) at a velocity v and denote the kinetic energy change associated with it by $\Delta \mathcal{E}_k$. We then assume that a mass per unit thickness $\mathcal{M} \sim \rho \ell^2$, where ρ is the mass density, attains a velocity that scales with v. Therefore, we can estimate

$$\Delta \mathcal{E}_k \sim \beta \frac{1}{2} \mathcal{M} v^2 \sim \frac{1}{2} \beta \rho \, \ell^2 v^2 \ , \tag{13.15}$$

where β is a dimensionless number. Note that $\Delta \mathcal{E}_k > 0$, i.e., the crack radiates kinetic energy that has to be supplied by the stored elastic energy. For reasons that will become clear immediately,

we denote the energy change in Eq. (13.11) as $\Delta\mathcal{E}_{qs}$, where the subscript stands for "quasi-static", and write

$$\Delta\mathcal{E}_{qs}(\ell) = \Delta\mathcal{E}_{qs}(\ell_c) - \alpha\frac{\sigma^2}{2E}(\ell - \ell_c)^2 \ . \tag{13.16}$$

Therefore, we have for the total change of energy associated with crack motion the following relation

$$\Delta\mathcal{E}_{tot}(\ell) = \Delta\mathcal{E}_s(\ell) + \Delta\mathcal{E}_p(\ell) + \Delta\mathcal{E}_k(\ell) \sim \Delta\mathcal{E}_{qs}(\ell_c) - \alpha\frac{\sigma^2}{2E}(\ell - \ell_c)^2 + \frac{1}{2}\beta\rho\,\ell^2 v^2 \ . \tag{13.17}$$

The next key point is to note that when $\ell > \ell_c$, the process becomes highly dynamic, i.e. the crack experiences rapid acceleration, and hence there is no time for energy to flow in and/or out of the system. Consequently, we approximately have $\Delta\mathcal{E}_{tot}(\ell) \simeq \Delta\mathcal{E}_{qs}(\ell_c)$ (i.e. energy may change form — surface, kinetic and potential — but the sum is fixed). Substituting this relation in the above equation and solving for $v(t) = \dot{\ell}(t)$, we obtain the following evolution equation for the crack's length $\ell(t)$

$$\dot{\ell}(t) \simeq v_{max}\left(1 - \frac{\ell_c}{\ell(t)}\right) \ , \tag{13.18}$$

where

$$v_{max} \equiv \sqrt{\frac{\alpha\,\sigma^2}{\beta\,E\,\rho}} \ . \tag{13.19}$$

This is a remarkably simple and insightful result; it tells us that under the prescribed conditions and when $\ell > \ell_c$ (obviously $v=0$ for $\ell \leq \ell_c$), the crack accelerates monotonically toward a limiting velocity v_{max}. Moreover, since this equation does not include $\dot{v}$ term it suggest that the crack tip may be regarded as a massless particle. The above argument does not tell us how exactly the limiting velocity v_{max} is related to intrinsic velocity scales in the system, e.g. the various elastic wave-speeds. In 1957 Stroh correctly argued that v_{max} should in fact be identified with the Rayleigh wave-speed c_R because in the limit of high speeds a crack should be viewed as a surface perturbation. This seems consistent with the idea that a crack tip should be regarded as a massless particle, in which case we expect it to propagate at the limiting velocity of the theory. This also suggests "relativistic" effects, that will be mentioned later.

This scaling theory that leads to Eq. (13.18) is due to Sir Nevill Mott (1947), who was awarded the Nobel prize in Physics in 1977 for his work on the electronic structure of disordered solids (he also made seminal contributions to the theory of fragmentation and other important problems). As it sometimes happens in the history of science, great scientists obtain essentially correct results even though they make fundamental physical mistakes. In the present case, the analysis did not take into account the fact that cracks induce *singular* stress fields and the kinetic and potential

energies actually diverge as the propagation speed approaches the limiting velocity – the Rayleigh wave-speed c_R. However, the final result depends only on the ratio of the two, which exhibit the same divergence and hence cancels out. It took about 30 years and serious mathematical developments to actually properly derive Eq. (13.18), including c_R as v_{max}. We might get a glimpse at this towards the end of the course.

Before we proceed to make things more accurate and quantitative, let us note that it is conventional to specify three modes of fracture, defined through the symmetry of the loading conditions with respect to a crack. Mode I fracture corresponds to tensile loading, i.e. tensile stresses that act perpendicularly to the crack faces, and is characterized by the following symmetry properties of a two-dimensional (in-plane) vectorial displacement field $\boldsymbol{u} = (u_x, u_y, 0)$

$$u_x(x, -y) = u_x(x, y) ,$$
$$u_y(x, -y) = -u_y(x, y) . \tag{13.20}$$

Mode II fracture corresponds to shear loading, i.e. shear stresses that act parallel to the crack faces, and is characterized by the following symmetry properties of a two-dimensional (in-plane) vectorial displacement field $\boldsymbol{u} = (u_x, u_y, 0)$

$$u_x(x, -y) = -u_x(x, y) ,$$
$$u_y(x, -y) = u_y(x, y) . \tag{13.21}$$

Mode III fracture corresponds to anti-plane shear loading and is characterized by the following symmetry properties of a two-dimensional (out-of-plane) scalar displacement field $\boldsymbol{u} = (0, 0, u_z)$

$$u_z(x, -y) = -u_z(x, y) . \tag{13.22}$$

B.   Rigorous results in the framework of Linear Elastic Fracture Mechanics

Up to now we used various scaling arguments to gain insight into the nature of cracks and the fracture process. We did not, however, touch upon the most striking feature of cracks, i.e. the existence of near tip singularity. We stress again that even though fracture is a strongly nonlinear and dissipative phenomenon, we presently focus on the linear elastic aspects of fracture phenomena, in the framework of the so-called Linear Elastic Fracture Mechanics (LEFM).

Inglis solution

Our story should start with the solution of Inglis (1913). Inglis considered a two-dimensional elliptical hole of major and minor axes a and b, respectively, inside an infinite linear elastic solid loaded by a remote tensile stress σ^∞ perpendicularly to the major axis of the hole. Inglis solved the complete problem analytically, but his main result can be presented in a compact manner. Denote the maximal tensile stress along the hole by σ_{max}, then

$$\frac{\sigma_{max}}{\sigma^\infty} = 1 + \frac{2a}{b} \ . \tag{13.23}$$

For a circular hole, $a = b$, we obtain a mild amplification factor, $\sigma_{max} = 3\,\sigma^\infty$. However, when the hole becomes more and more elongated the amplification factor increases. When it approaches a crack, $b/a \to 0$, the stress diverges. We therefore see that the geometry of defects plays a big role in determining the strength of materials and that cracks concentrate enormous stresses near their tips, i.e. cracks are stress amplifiers. It is this physical effect that explains the dramatic difference between the theoretical and practical strength of solids. The Inglis analysis has very practical implications; if you have a crack in your structure, you would better drill a hole at its tip to increase its radius of curvature. Engineers do that and now you understand why, even though it might appear counterintuitive to the layman. The Inglis solution played an important role in the development of fracture theory. In fact, Griffith was aware of the Inglis solution and used it to derive his famous 1922 result, Eq. (13.13), including all pre-factors.

Williams eigenfunctions expansion

Our next stop would be in the 1950's (there are good reasons why it happened in the 1950's, I will comment about this in class), with the so-called Williams expansion. Consider a linear elastic solid under quasi-static conditions, for which we have

$$\nabla^2 \nabla^2 \chi(r,\theta) = \left(\partial_{rr} + r^{-1}\partial_r + r^{-2}\partial_{\theta\theta}\right)^2 \chi(r,\theta) = 0 \ . \tag{13.24}$$

where $\chi(r,\theta)$ is the Airy stress potential. Let us look for a solution of the form $\chi(r,\theta) = r^{\lambda+2} f(\theta)$ (you already know from previous discussions that there are more solutions, e.g. $\log r$). Operating with ∇^2 on this Ansatz, we obtain

$$\left(\partial_{rr} + r^{-1}\partial_r + r^{-2}\partial_{\theta\theta}\right) r^{\lambda+2} f(\theta) = r^\lambda \left[(\lambda+2)^2 + \frac{d^2}{d\theta^2}\right] f(\theta) \equiv r^\lambda g(\theta) \ . \tag{13.25}$$

Operating with ∇^2 again yields

$$\left(\partial_{rr} + r^{-1}\partial_r + r^{-2}\partial_{\theta\theta}\right) r^\lambda g(\theta) = r^{\lambda-2} \left[\lambda^2 + \frac{d^2}{d\theta^2}\right] g(\theta) = 0 \ , \tag{13.26}$$

and therefore we end up with the following ordinary differential equation

$$\left[\lambda^2 + \frac{d^2}{d\theta^2}\right]\left[(\lambda+2)^2 + \frac{d^2}{d\theta^2}\right]f(\theta) = 0 \ . \tag{13.27}$$

Assume then a solution of the form $f(\theta) = e^{\alpha\theta}$, which leads to the following algebraic equation

$$\left[\lambda^2 + \alpha^2\right]\left[(\lambda+2)^2 + \alpha^2\right] = 0 \ . \tag{13.28}$$

The solution is

$$\alpha_{1,2} = \pm i\lambda \quad \alpha_{1,2} = \pm i(\lambda+2) \ , \tag{13.29}$$

therefore

$$f(\theta) = a\cos(\lambda\theta) + b\cos[(\lambda+2)\theta] + c\sin(\lambda\theta) + d\sin[(\lambda+2)\theta] \ . \tag{13.30}$$

To determine the parameters we need to introduce a crack. Consider then a straight mode I crack where (r,θ) represents a coordinate system attached to the tip and $\theta = 0$ points in the direction of the tangent to the crack tip. Symmetry alone, $f(\theta) = f(-\theta)$, implies $c = d = 0$. As we explained above, a crack is introduced mathematically as traction-free boundary conditions of the form

$$\sigma_{\theta\theta}(r,\theta{=}\pm\pi) = \partial_{rr}\chi(r,\theta{=}\pm\pi) = 0, \quad \sigma_{r\theta}(r,\theta{=}\pm\pi) = -\partial_r\left(r^{-1}\partial_\theta\chi(r,\theta{=}\pm\pi)\right) = 0 \ . \tag{13.31}$$

Using $\chi(r,\theta) = r^{\lambda+2}\left(a\cos(\lambda\theta) + b\cos[(\lambda+2)\theta]\right)$, we obtain

$$\sigma_{\theta\theta}(r,\theta) = (\lambda+2)(\lambda+1)r^\lambda\left(a\cos(\lambda\theta) + b\cos[(\lambda+2)\theta]\right) \ , \tag{13.32}$$

$$\sigma_{r\theta}(r,\theta) = (\lambda+1)r^\lambda\left(a\lambda\sin(\lambda\theta) + (\lambda+2)b\sin[(\lambda+2)\theta]\right) \ . \tag{13.33}$$

Applying the boundary conditions, we obtain

$$(a+b)\cos(\lambda\pi) = 0 \ , \tag{13.34}$$

$$[a\lambda + b(\lambda+2)]\sin(\lambda\pi) = 0 \ . \tag{13.35}$$

Denoting $n = 0, \pm1, \pm2, ...$, the solution reads

$$\lambda = n \qquad \Longrightarrow \qquad b = -a \ , \tag{13.36}$$

$$\lambda = \frac{2n+1}{2} \qquad \Longrightarrow \qquad b = -\frac{a\lambda}{\lambda+2} \ . \tag{13.37}$$

We therefore end up with the Williams eigenfunctions expansion

$$\sigma_{ij}(r,\theta) = \sum_{m=-\infty}^{m=\infty} a_m r^{m/2} f_{ij}^{(m)}(\theta) \ , \tag{13.38}$$

where $f_{ij}^{(m)}(\theta)$ are explicitly expressed in terms of trigonometric functions as above. An immediate striking feature here is that the expansion contains half-integer powers. These emerge from the fact that a crack introduces a discontinuity in the fields, i.e. a crack is regarded as a mathematical branch cut.

What can we say about $\{a_m\}$? How can one calculate them? It is crucial to understand that we *did not* consider the outer boundary conditions of the problem, i.e. we essentially performed a crack tip asymptotic expansion, without even formulating the global boundary-value problem. $\{a_m\}$ are determined from the solution of each specific global boundary-value problem, which in general cannot be done analytically. The Williams expansion in Eq. (13.38) is therefore universal, independent of the external geometry and boundary conditions. The asymptotic expansion of course has a finite radius of convergence typically determined by some geometric properties of the crack, e.g. length for straight cracks or curvature for non-straight ones (note that we imposed the boundary conditions at $\theta = \pm\pi$, assuming that on the scale of interest any path curvature can be neglected).

Universal singular crack tip fields

The next question we would like to ask ourselves is whether all m's in the Williams expansion in Eq. (13.38) are physically acceptable? The point is the following: all terms with $m < -1$ will lead to *unbounded* linear elastic strain energy in the $r \to 0$ limit. To see this, recall that in a linear theory we have $\boldsymbol{\varepsilon} \sim \boldsymbol{\sigma} \sim r^{m/2}$ and hence the strain energy density scales as $\frac{1}{2}\sigma_{ij}\varepsilon_{ij} \sim r^m$. Therefore, the energy per unit thickness reads $\int \frac{1}{2}\sigma_{ij}\varepsilon_{ij}\, r\, dr\, d\theta \sim \int r^{m+1} dr$. It diverges in the $r \to 0$ limit for $m < -1$ (more precisely, we are interested in the energy flux into the tip region when the crack advances incrementally, which in fact does not involve integration over r, as will be discussed below). We should therefore rewrite Eq. (13.38) as

$$\sigma_{ij}(r,\theta) = \sum_{m=-1}^{m=\infty} a_m r^{m/2} f_{ij}^{(m)}(\theta) \ . \tag{13.39}$$

The above discussion has serious implications. As we have included the $m = -1$ term in the expansion, it seems as if we allow the stress tensor to diverge in the $r \to 0$ limit as long as it results in an integrable elastic energy. This divergence is precisely the one we discussed in the context of the Inglis solution above. Obviously a physical quantity such as the stress cannot really diverge, i.e. there must be some small scale physical regularization of the divergence. However,

the square-root singular spatial variation of the stress (and strain) field near the tip of a crack is real and of enormous importance. We already understood that it is this singularity that essentially explains the huge discrepancy between the theoretical and practical strength of materials.

In 1957 Irwin made the next seminal contribution. He pointed out that the series in Eq. (13.39) is dominated by the $m = -1$ term as the crack tip is approached, $r \to 0$. He therefore focussed on this contribution, for which we have $\lambda = -1/2$ and $b = -a\lambda/(\lambda + 2) = a/3$ in Eq. (13.32), leading to

$$\sigma_{\theta\theta}(r, \theta) = \frac{a}{4\sqrt{r}} \left[3\cos\left(\frac{\theta}{2}\right) + \cos\left(\frac{3\theta}{2}\right) \right] = \frac{a}{\sqrt{r}} \cos^3\left(\frac{\theta}{2}\right) . \tag{13.40}$$

Irwin defined $a \equiv K_I/\sqrt{2\pi}$, where K_I is known as the mode I stress intensity factor (the other symmetry modes have their own stress intensity factors). It is a fundamental quantity in the theory of fracture as it quantifies the intensity of the near tip singularity. It has rather strange physical dimensions of stress times square-root of length. Before we continue to discuss it, we note that for $\theta = 0$ we have

$$\sigma_{\theta\theta}(r, 0) = \sigma_{yy}(r, 0) = \frac{K_I}{\sqrt{2\pi r}} , \tag{13.41}$$

which directly quantifies the strength of the tensile stress that tends to drive the crack into motion. The other two components of the stress field corresponding to the $m = -1$ term are easily obtained and read

$$\sigma_{r\theta}(r, \theta) = \frac{K_I}{\sqrt{2\pi r}} \cos^2\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) , \tag{13.42}$$

$$\sigma_{rr}(r, \theta) = \frac{K_I}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right) \left[1 + \sin^2\left(\frac{\theta}{2}\right) \right] . \tag{13.43}$$

This asymptotic stress field $\boldsymbol{\sigma}$ is termed the "K-field".

The emerging mathematical and physical picture is neat. Whatever external geometry and boundary conditions we have, the near crack tip fields are *universal* and characterized by a square-root singularity. All the information about the large scales is transmitted to the crack tip region by a single number, the stress intensity factor K_I – the only non-universal quantity in the universal K-field (if mode II and III loadings are relevant, we have two additional universal fields, all feature a square-root divergence, and two additional stress intensity factors, K_{II} and K_{III}). As we stressed above, calculating it entails the solution of the global crack problem. In the case of a single straight crack of length ℓ in an infinite medium loaded by a tensile stress σ^∞ at infinity (an Inglis crack), dimensional analysis implies that $K_I \sim \sigma^\infty \sqrt{\ell}$ and only the order unity prefactor should be calculated from the exact global solution.

As we explained above, there must be some physical regularization of the singularity at small scales, which means that nonlinear and dissipative processes (e.g. plasticity) are taking place near the tip of crack relax the stress. Therefore, the K-field should be in fact interpreted as "intermediate asymptotics" separating the large ("outer") scales linear elastic behavior from the small ("inner") scales nonlinear and dissipative behavior. A crucial assumption here is that we indeed have scales separation, i.e. that linear elasticity is valid everywhere except for a region near the crack tip – the so-called "process zone" – whose dimensions are much smaller than any other lengthscale in the crack problem. This assumption is termed "small scale yielding" (though the nonlinear and dissipative processes near the tip are not necessarily or exclusively plastic yielding and deformation). It is important to stress again that the ("inner") scales near the tip of the crack, where fracture is actually taking place, are always subjected to universal boundary conditions in the form of the K-field and that the specific properties of a given problem at the larger ("outer") scales are transmitted to the tip region only through the stress intensity factor. It is this scales separation that makes a linear elastic approach so useful. Fracture is a physical phenomenon that exhibits a rather unique coupling between widely different scales. It is also a natural laboratory for extreme out-of-equilibrium physics that takes place near the tip region even if external loading conditions are mild.

Crack tip opening displacement (CTOD)

Let us explore some more consequences of the universal K-field in Eqs. (13.40), (13.42) and (13.43). First, we use Hooke's law to transform this stress field into a displacement field. The result reads (derive)

$$u_x(r, \theta) = \frac{K_I \sqrt{r}}{4\mu\sqrt{2\pi}} \left[(2\kappa - 1) \cos\left(\frac{\theta}{2}\right) - \cos\left(\frac{3\theta}{2}\right) \right], \tag{13.44}$$

$$u_y(r, \theta) = \frac{K_I \sqrt{r}}{4\mu\sqrt{2\pi}} \left[(2\kappa + 1) \sin\left(\frac{\theta}{2}\right) - \sin\left(\frac{3\theta}{2}\right) \right], \tag{13.45}$$

where

$$\kappa = \begin{cases} \frac{3 - \nu}{1 + \nu} & \text{for plane-stress ,} \\ 3 - 4\nu & \text{for plane-strain .} \end{cases} \tag{13.46}$$

We now ask the following question: what is the shape of the crack tip when it opens up under external loadings, i.e. what is the crack tip opening displacement? To answer this question we would be interested in calculating the dependence of $\varphi_x(r, \pi)$ on $\varphi_y(r, \pi)$, where $\boldsymbol{\varphi} = \boldsymbol{x} + \boldsymbol{u}$ is the

motion (recall that in the linear theory we do not distinguish between the undeformed $\boldsymbol{X}$ and the deformed $\boldsymbol{x}$ coordinates). We then have

$$\varphi_x(r, \pi) = r\cos(\pi) + u_x(r, \pi) = -r \ , \tag{13.47}$$

$$\varphi_y(r, \pi) = r\sin(\pi) + u_y(r, \pi) \sim \frac{K_I}{\mu}\sqrt{r} \ . \tag{13.48}$$

Therefore, we obtain

$$\varphi_x(r, \pi) \sim -\frac{\mu^2}{K_I^2}\varphi_y^2(r, \pi) \ , \tag{13.49}$$

which implies that the crack tip opening displacement is *parabolic*. The curvature of the parabola is determined by μ^2/K_I^2.

C.   Configurational forces and the J-integral

Up to now we discussed the linear elastic fields near the tip of the crack. But we have not touched upon the question of how fracture actually happens; What drives it? When does it happen? To start answering these questions, let us introduce the concept of configurational forces, a fundamental concept in non-equilibrium continuum physics. Unfortunately, we cannot discuss this concept in great detail, but rather sketch the basic ideas. Configurational forces are very general and useful physical objects; in fact, we already ran into them in the context of dislocations, where the configurational force is termed the Peach-Köhler force. The basic idea and formalism were laid down by Eshelby who introduced the concept of a generalized force acting on a defect by realizing that defects break some basic symmetry in a given physical system. He derived an elastic energy-momentum tensor, where one or more of the components are not conserved due to the presence of a defect. These configurational forces are thermodynamic forces acting on symmetry-breaking defects, to be distinguished from Newtonian forces that act on particles. To convey the basic idea let us assign to a defect (e.g. a dislocation or a crack) a coordinate ℓ and write down the total rate of dissipation (per unit thickness) Φ associated with the defect motion as

$$\Phi = -\frac{\partial\mathcal{E}}{\partial\ell}\dot{\ell} \geq 0 \ , \tag{13.50}$$

where $\mathcal{E}$ is the energy (per unit thickness) stored in the loading device and the system. The configurational (generalized) force G acting on the defect is defined as

$$G \equiv -\frac{\partial\mathcal{E}}{\partial\ell} \ . \tag{13.51}$$

Note that since the inequality in (13.50) is a dissipation (second law) inequality, we see that the configurational (generalized) force G and the defect coordinate ℓ are thermodynamically conjugate such that the product $G\dot{\ell}$ is the dissipation (compare to other dissipation inequality we have encountered, e.g. $\boldsymbol{\sigma}:\dot{\boldsymbol{\epsilon}}^{pl} \geq 0$). It also shows that $G = 0$ in the absence of dissipation. G has the dimensions of energy per unit area. Let us understand what the physical meaning of G is when the defect is a crack (without following the energy-momentum tensor derivation). G is associated with energy dissipation, yet it is obtained by the variation of the total elastic energy (stored in both the loading device and the system) with respect to the crack tip coordinate. Since dissipation takes place only at the crack tip, this means that G quantifies the energy that flows from the loading and the elastic bulk into the singularity where it dissipates.

With this physical understanding we can write down an expression for G. Consider a crack moving with an instantaneous speed v (which may vary with time) in the x-direction and a contour $\mathcal{C}$ that starts at one crack face and ends at the other one that translates with the crack tip. Let us express the energy flux through the contour $\mathcal{C}$. This flux is composed of two physically distinct contributions. The first is the rate of work the tractions acting on $\mathcal{C}$ do on the material inside $\mathcal{C}$. Had $\mathcal{C}$ been a fixed material line, that would be the only contribution to the energy flux. However, as $\mathcal{C}$ is translating with the crack tip, energy flows through $\mathcal{C}$ also due to the transport of material (which carries potential and kinetic energies) through $\mathcal{C}$. Put together we have

$$J(\mathcal{C}) = \int_{\mathcal{C}} \left[s_{ij} \frac{\partial u_i}{\partial t} n_j + (U + T)\, v n_x \right] ds \;, \tag{13.52}$$

where $\boldsymbol{n}$ is an outward unit normal on $\mathcal{C}$, $\boldsymbol{s}$ is the first Piola-Kirchhoff stress tensor, ds is an infinitesimal arclength element along $\mathcal{C}$ and

$$T = \frac{\rho}{2} \frac{\partial u_i}{\partial t} \frac{\partial u_i}{\partial t}, \quad U = \int_{-\infty}^{t} s_{ij} \frac{\partial^2 u_i}{\partial x_j \partial t'} dt' \;. \tag{13.53}$$

are the kinetic and potential energy densities, respectively. The line integral is understood to be taken in the counterclockwise direction. This in fact can be shown to be an integral over one component of the elastic energy-momentum tensor. We note that all quantities and coordinates refer to the reference configuration (for the simplicity of the notation we did not use the $\boldsymbol{X}$'s as we did earlier in the course) and that U is *any* elastic strain energy function (possibly nonlinear). The integral in Eq. (13.52), which is sometimes termed the J-integral, quantifies the instantaneous rate of energy flow through $\mathcal{C}$ towards the crack tip.

The dimensions of J-integral, energy per unit length per unit time, are different from those of

G above. Obviously the two are related through the crack speed v such that

$$G = \lim_{\mathcal{C} \to 0} \frac{J(\mathcal{C})}{v} = \lim_{\mathcal{C} \to 0} \left[\frac{1}{v} \int_{\mathcal{C}} \left[s_{ij} \frac{\partial u_i}{\partial t} n_j + (U + T) v n_x \right] ds \right] . \tag{13.54}$$

G, the configurational (generalized) force discussed above, is termed in the present context the "dynamic energy release rate" (though it is not an energy rate, but rather an energy per unit area). Was it necessary to take the limit $\mathcal{C} \to 0$? i.e. why couldn't we simply have $G = J/v$? The point is that in order for G to be a fundamental physical quantity it must be *independent* of the path (contour) $\mathcal{C}$. This is not true in general if $\mathcal{C}$ can be anywhere inside the elastic bulk. However, it is independent of $\mathcal{C}$ if the latter is taken within the universal singular region where the K-field is dominant (we do not prove this here), which is ensured if $\mathcal{C}$ is sufficiently small.

There is one important class of situations in which G (and J) are independent of the path (contour) $\mathcal{C}$ for *any* $\mathcal{C}$, irrespective if it is inside or outside the universal singular region. This happens for steady state crack propagation, i.e. when v is time-independent. Let us prove it. We start with the equations of motion

$$\frac{\partial s_{ij}}{\partial x_j} = \rho \frac{\partial^2 u_i}{\partial t^2} , \tag{13.55}$$

where s_{ij} are the component of the first Piola-Kirchhoff stress tensor, ρ is the mass density in the reference (undeformed) configuration, u_i are the components of the displacement vector and x_j are the reference (undeformed) coordinates.

We multiply Eq. (13.55) by $\dot{u}_i$ and sum over the index i

$$\frac{\partial s_{ij}}{\partial x_j} \frac{\partial u_i}{\partial t} = \rho \frac{\partial u_i}{\partial t} \frac{\partial^2 u_i}{\partial t^2} , \tag{13.56}$$

which implies

$$\frac{\partial}{\partial x_j} \left(s_{ij} \frac{\partial u_i}{\partial t} \right) - s_{ij} \frac{\partial^2 u_i}{\partial x_j \partial t} = \rho \frac{\partial u_i}{\partial t} \frac{\partial^2 u_i}{\partial t^2} , \tag{13.57}$$

which implies

$$\frac{\partial}{\partial x_j} \left(s_{ij} \frac{\partial u_i}{\partial t} \right) = \frac{\partial}{\partial t} (U + T) . \tag{13.58}$$

The crucial point is that for steady state propagation we have

$$\partial_t = -v \partial_x , \tag{13.59}$$

for which we have

$$G = \int_{\mathcal{C}} \left[(U + T) n_x - s_{ij} \frac{\partial u_i}{\partial x} n_j \right] ds . \tag{13.60}$$

We should prove that the latter is independent of $\mathcal{C}$. For that aim, consider a *closed path* ∂A such that two segments of the path lie along the two crack faces. Denoting the area enclosed in ∂A by A, the proof is as follows

$$\int_{\partial A} (U+T)\, n_x ds = \int_A \frac{\partial}{\partial x}(U+T)\, dA = -v^{-1} \int_A \frac{\partial}{\partial t}(U+T)\, dA = -v^{-1} \int_A \frac{\partial}{\partial x_j}\left(s_{ij}\frac{\partial u_i}{\partial t}\right) dA$$
$$= \int_A \frac{\partial}{\partial x_j}\left(s_{ij}\frac{\partial u_i}{\partial x}\right) dA = \int_{\partial A} s_{ij}\frac{\partial u_i}{\partial x} n_j ds \ , \tag{13.61}$$

where Eqs. (13.58)-(13.59) and the divergence theorem were used. This implies

$$\int_{\partial A}\left[(U+T)\, n_x - s_{ij}\frac{\partial u_i}{\partial x} n_j\right] ds = 0 \ , \tag{13.62}$$

which completes the proof. To see this, recall that the two segments that lie along the crack faces do not contribute to the integral in Eq. (13.62) because there we have $n_x = 0$ and $s_{ij}n_j = 0$ (the latter due to the traction-free boundary conditions). This implies that the sum of the two line integrals over the two remaining portions of the path vanishes. However, the direction of integration is reversed in one of them (such that the path is closed). If we reverse it back to be counterclockwise, we get a minus sign that immediately implies that for every path that starts at the lower crack face, encircles the tip in the counterclockwise direction and ends at the upper crack face, the value of the integral is the same.

In particular, this result is valid for quasi-static cracks. Though the ideas about configurational forces were developed by Eshelby in the early 1950's, the integral discussed above in the context of fracture theory was independently derived by Cherepanov (1967) and Rice (1968) for quasi-static cracks and then extended to the dynamic case in the 1970's.

D. Fracture toughness and fracture energy

We are now in a position to ask what is the criterion for crack initiation and motion. From the perspective of LEFM, there are two interrelated approaches; the first one asserts that a crack starts to propagate when the stress intensity factor K_I surpasses a critical value K_{I_C}, the so-called "fracture toughness". This is a very useful concept, which translates into a fundamental material property of great practical importance. The practice is rather simple: a crack is introduced into a sample of prescribed geometry. Then the sample is loaded following a prescribed protocol until it fails and the critical loading condition is tracked. The stress intensity factor K_I is calculated numerically for the prescribed geometry and loading, as a function of the loading parameter. K_{I_C}

is the value of K_I at the critical loading conditions. The engineer can then select materials with a given fracture toughness K_{I_C}, depending on the application. Metals, such as those used to build your car, can reach K_{I_C} of tens or even $100 \ \text{MPa}\sqrt{\text{m}}$. Very brittle materials, such as your window glass, are characterized by K_{I_C} which is smaller than $1 \ \text{MPa}\sqrt{\text{m}}$. It worthwhile mentioning that we usually want materials to be stiff, i.e. to deform as little as possible when they perform, and also to be tough, i.e. to resist crack propagation and failure. Unfortunately, these properties are usually inversely related. In fact, Nature does it quite well (think of your teeth or your bones) and these days we see intense research activity in which people try to mimic natural design principles to create better materials. This scientific strategy is called "biomimetics".

When $K_I < K_{I_C}$ the crack remains stationary/static. For $K_I \geq K_{I_C}$ motion sets in and $\dot{\ell} = v > 0$. Under these conditions, the stress intensity factor needed to propagate a crack at a speed v is termed the "dynamic fracture toughness", $K_{I_C}^d$.

The other approach to characterize the fracture resistance of materials is based on energy considerations. Above, we have expressed the energy flux into the crack tip/sigularity in terms of the near tip fields. From the perspective of LEFM this energy flows into the singularity which acts as an energy sink, where energy is being dissipated by highly localized and nonlinear processes. The amount of energy per unit crack area that should be supplied to the tip in order to propagate at a speed v is denoted by $\Gamma(v)$. It is known as the "fracture energy". This material property is extremely difficult to predict theoretically, because it lumps together physical processes that take place under extreme conditions at the small scales near the tip of a crack. Using Eq. (13.54), we obtain the following energy balance at the crack tip

$$G = \Gamma(v) \ . \tag{13.63}$$

When $\Gamma(v)$ is known and G is calculated in terms of the crack length (if the crack is assumed to be straight), this becomes an equation of motion for the crack tip. Under certain conditions Mott's scaling prediction in Eq. (13.18) is recovered, where v_{max} is replaced with c_R. It is crucial to understand that the two sides of Eq. (13.63) have a fundamentally different status. The left hand side is a quantity that can be calculated from the linear elastic solution for a given crack configuration and speed. It quantifies the amount of linear elastic energy flowing from the large scales into the small scales near the crack tip. The right hand side quantifies the amount of energy being dissipated per unit crack area in the small scales near the tip when the crack propagates at a speed v. We are talking here about fundamentally different physics that requires completely different theoretical frameworks. Crack initiation is characterized by $\Gamma(v)$ when $v \to 0$. This is

sometimes denoted as Γ_c or G_c. Unfortunately, as we mentioned above, typically we do not know how to calculate $\Gamma(v)$ from first principles. In fact, Eq. (13.63) is used in order to measure $\Gamma(v)$. This is a theory assisted (because the left hand side can be calculated) measurement. The same practice is followed to measure K_{I_C}, as explained above.

The fracture energy $\Gamma(v)$ is a generalization of the concept of surface energy γ. The latter quantifies the amount of energy needed in order to break molecular bonds per unit area. We already estimated γ to be of the order of 1 J/m² for ordinary materials. $\Gamma(v)$, on the other hand, refers to the dynamical process that creates new surfaces, which might be different because it may involve additional dissipative processes that are triggered by the large stresses and strains near the crack tip. In general, 2γ (the two appears because we are creating two surfaces) is the lower, velocity-independent, bound of $\Gamma(v)$

$$\Gamma(v) = 2\gamma + \text{additional crack tip dissipation per unit crack area} . \qquad (13.64)$$

The latter includes visco-elasticity, plasticity, damage (voids, micro-cracking) etc. Can these dissipative processes make a significant contribution to $\Gamma(v)$? In nearly ideally brittle materials like window glass, the major dissipative process is bond breaking and we have $\Gamma \simeq 2\gamma$. However, for many other brittle materials this is *not* the case. Think for example about Plexiglass (Perspex) or Polycarbonate (the material from which your glasses are made of). These are glassy polymers. In order to break monomers – which still costs about 1 J/m² – you need first to disentangle the polymeric chains and to slide them one against the other, which involves quite a lot of energy dissipation, much more than 1 J/m². Therefore, for such materials, even though dissipation is localized near the crack tip, the fracture energy may be *orders of magnitude* bigger than γ.

Finally, we should ask whether the two ways described above to quantify the fracture resistance of solids, the fracture toughness K_{I_C} and the fracture energy Γ are related. The answer is yes. To see this we should consider the J-integral in Eq. (13.54) and use the asymptotic K-field to evaluate it. We have not calculated the K-field in the dynamic case (this will be done for mode III cracks below), but here we focus only on the essential features of the outcome. The crucial point to notice is that all the terms in the integrand are quadratic in the strain (i.e. appear as products of the strain and stress). Since both the stress and strain scale as $K_I/\sqrt{r}$, the integrand scales as (with the correct dimensions) K_I^2/Er. When multiplied by $ds = rd\theta$, we obtain (as discussed explicitly above in the context of the Williams expansion), a finite energy release

$$G \sim \frac{K_I^2}{E} . \qquad (13.65)$$

This is a very important result that tells us that saying that G should meet a threshold is equivalent to saying that K_I should meet a threshold. The prefactor is indeed order unity for quasi-static cracks, $v \to 0$, but is a universal and highly nontrivial function for finite v. In fact, it diverges as $v \to c_R$. We will not discuss this here (see tutorial).

E. Dynamic fracture

Our goal here is to better understand dynamic effects in fracture mechanics. For that aim, in order to simplify the mathematical development, we focus on mode III fracture which is described by scalar elasticity

$$\mu \nabla^2 u_z(x_1, x_2, t) = \rho \partial_{tt} u_z(x_1, x_2, t) . \tag{13.66}$$

Define then a coordinate system moving with the crack tip

$$x(x_1, x_2, t) = x_1 - \ell(t) , \tag{13.67}$$

$$y(x_1, x_2, t) = x_2 , \tag{13.68}$$

where $\ell(t)$ is the crack tip position (the crack is assumed be to straight, but all of the results remain the same for a curved trajectory). We therefore have

$$u_z(x_1, x_2, t) = w(x, y, t) . \tag{13.69}$$

We would like now to express Eq. (13.66) as an equation for $w(x, y, t)$, which reads

$$\partial_{xx} w + \partial_{yy} w = \frac{1}{c_s^2} \left[\partial_{xx} w \, \dot{x}^2 + \partial_x w \, \ddot{x} + 2 \partial_{xt} w \, \dot{x} + \partial_{tt} w \right] . \tag{13.70}$$

Note that a partial derivative of u_z with respect to t is different from a partial derivative of w with respect to t, because in the former x_1 and x_2 are fixed and in the latter x and y are fixed. Recalling that $\dot{x} = -\partial_t \ell(t) = -v$, we actually have

$$\partial_{xx} w + \partial_{yy} w = \frac{1}{c_s^2} \left[v^2 \partial_{xx} w - \dot{v} \partial_x w - 2 v \partial_{xt} w + \partial_{tt} w \right] . \tag{13.71}$$

This shows, for example, how the crack tip acceleration $\dot{v}$ enters the equation of motion.

The next question we should address is which terms in the equation contribute to the leading singular field. From the energy considerations discussed above we know that the leading term in the near tip expansion behaves as $w \sim \sqrt{r}$ when $r \to 0$ and hence to leading order we have

$$\left(1 - \frac{v^2}{c_s^2} \right) \partial_{xx} w + \partial_{yy} w = 0 . \tag{13.72}$$

This shows explicitly that the crack tip acceleration does not contribute to leading order. Note also that the absence of explicit time derivatives here implies that as long as spatial derivatives are concerned we can use w and u_z interchangeably.

Let us solve this equation to leading order. Define

$$\alpha_s^2 = 1 - \frac{v^2}{c_s^2} \ , \tag{13.73}$$

which quantifies the "relativistic" change in length in the propagation direction. Then we have

$$\partial_{xx} w + \partial_{y'y'} w = 0 \ , \tag{13.74}$$

with

$$y' \equiv \alpha_s y = \sqrt{1 - \frac{v^2}{c_s^2}}\, y \ . \tag{13.75}$$

The relativistic effects (relative to the shear wave speed c_s) are already evident here with the appearance a Lorentz contraction which becomes strong at elastodynamic propagation velocities $(c \to c_s)$.

Eq. (13.74) is Laplace's equation, which we can readily solve using a complex functions technique that was discussed earlier in the course. For that aim define a complex variable ζ_s such that

$$\zeta_s = x + iy' = x + i\alpha_s y = r_s e^{i\theta_s} \ . \tag{13.76}$$

It would be more convenient to introduce polar coordinate system at the crack's tip

$$r = \sqrt{x^2 + y^2} \quad \text{and} \quad \theta = \tan^{-1}\left(\frac{y}{x}\right) \ . \tag{13.77}$$

We then have

$$r_s = r\sqrt{1 - \frac{v^2 \sin^2\theta}{c_s^2}} \quad \text{and} \quad \tan\theta_s = \alpha_s \tan\theta \ . \tag{13.78}$$

The solution to Eq. (13.74) is readily written as

$$w(\zeta_s) = \Im\left[f(\zeta_s)\right] \ , \tag{13.79}$$

where $f(\cdot)$ is an analytic function. The leading near tip contribution takes the form

$$f(\zeta_s) = a\,\zeta_s^{1/2} \ . \tag{13.80}$$

The boundary conditions read

$$\sigma_{zy}(r, \theta = \pm\pi) = 0 \ . \tag{13.81}$$

Let us calculate the stress components

$$\sigma_{zx} = \mu\partial_x w = \mu\Im\left[f'(\zeta_s)\right] = \mu\Im\left[\frac{a}{2}\zeta_s^{-1/2}\right] = -\frac{\mu a}{2}r_s^{-1/2}\sin\left(\frac{\theta_s}{2}\right), \tag{13.82}$$

$$\sigma_{zy} = \mu\partial_y w = \mu\Im\left[i\alpha_s f'(\zeta_s)\right] = \mu\Im\left[i\alpha_s\frac{a}{2}\zeta_s^{-1/2}\right] = \frac{\mu a}{2}\alpha_s r_s^{-1/2}\cos\left(\frac{\theta_s}{2}\right). \tag{13.83}$$

Since $\cos[\theta_s(\theta)/2]$ vanishes for $\theta = \pm\pi$, the boundary conditions in Eq. (13.81) are satisfied automatically.

The definition of the mode III stress intensity factor

$$K_{III} \equiv \lim_{r\to 0}\sqrt{2\pi r}\,\sigma_{zy}(r,\theta=0)\,, \tag{13.84}$$

implies

$$a = \frac{2K_{III}}{\mu\alpha_s\sqrt{2\pi}}\,. \tag{13.85}$$

Finally, we can write down the complete leading order solution

$$w(r,\theta) = \Im\left[a\,\zeta_s^{1/2}\right] = \frac{2K_{III}}{\mu\alpha_s\sqrt{2\pi}}r_s^{1/2}\sin\left(\frac{\theta_s}{2}\right), \tag{13.86}$$

and

$$\sigma_{zx}(r,\theta) = -\frac{K_{III}}{\alpha_s\sqrt{2\pi r_s}}\sin\left(\frac{\theta_s}{2}\right), \tag{13.87}$$

$$\sigma_{zy}(r,\theta) = \frac{K_{III}}{\sqrt{2\pi r_s}}\cos\left(\frac{\theta_s}{2}\right)\,. \tag{13.88}$$

We can also calculate the leading asymptotic contribution to the particle velocity

$$\dot{u}_z = \partial_t u_z(x_1,x_2,t)|_{x_1,x_2} = \partial_t w(x_1-\ell(t),x_2) = -v\partial_x w = -v\sigma_{zx}/\mu = \frac{vK_{III}}{\mu\alpha_s\sqrt{2\pi r_s}}\sin\left(\frac{\theta_s}{2}\right), \tag{13.89}$$

which features the same singular behavior. The results for the in-plane fracture modes (mode I and II) are qualitatively similar (e.g. they feature the same universal singularity), though they are more mathematically involved (see tutorial).

Dynamic fracture problems are extremely difficult to solve. Let us briefly explain why. From the perspective of Linear Elastic Fracture Mechanics (LEFM) the crack is regarded as boundary conditions. Enormous difficulties emerge from the fact that these boundary conditions are dynamic, i.e. they evolve in time. So unlike standard boundary value problems in which the domain is fixed, here the domain is evolving. The moving free boundary nature of dynamic fracture problems introduces serious nonlinearities into the problem. But there is a more serious issue here: The moving free boundary is *not* determined externally but rather should be solved for

self-consistently, i.e. the solution at time t determines the new boundary conditions at time $t+dt$. This is a remarkable mathematical feature. Worse than that is the fact that we do not know how the crack selects its path. LEFM does not tell us anything about that. Eq. (13.63) is a scalar energy balance equation that tells us that *if* $\Gamma(v)$ is known then the crack growth rate is known, but there is no information about the direction of growth. We will mention this again when we discuss the limitations of LEFM below. Finally, we would like to mention that dynamic fracture is extremely challenging from an experimental perspective. Take your window glass as an example. The size of the singular region is in the nanometer scale. The typical crack propagation speed is kilometers per second. It is impossible today, and most probably in the near future, to probe such lengthscales at such rates.

F. Limitations of Linear Elastic Fracture Mechanics (LEFM) and beyond it

While LEFM has revolutionized our understanding of the fracture of solids and has led to the development of a very successful engineering practice, it suffers from some serious limitations. In many cases, especially for metals (which are typically termed ductile), the small scale yielding assumption is not satisfied. Significant and spatially extended plastic deformation develops in the presence of a crack. This plastic deformation makes these materials tougher, but limits the usage of LEFM. For that aim, Elastic-Plastic Fracture Mechanics (EPFM) has been developed. Unfortunately, we cannot discuss it here.

LEFM is in fact not sufficient to properly describe fracture even in brittle materials in which the small scale yielding assumption is satisfied. To get a feeling of the problem, we will raise here two points. First, the asymptotic singular K-field of LEFM – while properly quantifying the flux of energy into the crack tip region – cannot actually tell us how things break. The quasi-static $(v \to 0)$ K-field in Eqs. (13.40), (13.42) and (13.43) has the following property

$$\sigma_{yy}(r, \theta{=}0; v{=}0) = \sigma_{xx}(r, \theta{=}0; v{=}0) \ . \tag{13.90}$$

(for $\theta = 0$, x can replace r and y can replace θ). For any $v > 0$ (see tutorial session) we have

$$\sigma_{yy}(r, \theta{=}0; v) < \sigma_{xx}(r, \theta{=}0; v) \ . \tag{13.91}$$

This is striking because it means that the material element whose unit normal points parallel (in the x-direction) to the crack will break before the material element whose normal points perpendicularly (in the y-direction) to the crack, which is of course the one that actually breaks

during mode I fracture. Therefore, the K-field cannot even explain why mode I cracks propagate as perpendicularly to the tensile loading. The inequality in (13.91) becomes stronger and stronger as v increases. This means that beyond some velocity (say, under plane-stress conditions)

$$\varepsilon_{yy} \sim \sigma_{yy} - \nu\sigma_{xx} \tag{13.92}$$

becomes negative, implying that compressive strains break the material under tension. This is of course wrong. These "puzzles" simply mean that the K-field is not the one that actually controls fracture, which takes place at smaller scales near the tip, and that even some qualitative features of it are not directly relevant.

The second point we raise concerns lengthscales. Experimental observations indicate that rapid straight cracks undergo all sorts of dynamic instabilities. These instabilities feature lengthscales that do not seem to be geometrical in nature. However, LEFM does not contain any intrinsic lengthscale and hence in principle cannot explain these instabilities. Moreover, as we mentioned above, LEFM does not tell us how a crack selects its path (direction), i.e. we still miss a physically well-established crack tip equation of motion. Without such an equation one cannot even think about asking questions regrading the stability of cracks, simply because there is no equation with which he can perform stability analysis. Some of these issues are currently investigated by physicists and other scientists working in the field.

Configurational forces

Consider a Lagrangian density

$$\mathcal{L}(u_i, \partial_j u_i, x_m) \ , \tag{13.93}$$

where the explicit appearance of x_m represents the breakdown of space homogeneity. The variation of $\mathcal{L}$ with x_l reads

$$\frac{\delta\mathcal{L}}{\delta x_l} = \frac{\partial\mathcal{L}}{\partial u_i}\partial_l u_i + \frac{\partial\mathcal{L}}{\partial(\partial_j u_i)}\frac{\partial(\partial_j u_i)}{\partial x_l} + \left(\frac{\partial\mathcal{L}}{\partial x_l}\right)_{expl} . \tag{13.94}$$

Noting that

$$\frac{\partial(\partial_j u_i)}{\partial x_l} = \frac{\partial^2 u_i}{\partial x_j \partial x_l} = \frac{\partial(\partial_l u_i)}{\partial x_j} \tag{13.95}$$

and

$$\frac{\partial\mathcal{L}}{\partial(\partial_j u_i)}\frac{\partial(\partial_l u_i)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\partial\mathcal{L}}{\partial(\partial_j u_i)}\partial_l u_i\right) - \left(\frac{\partial}{\partial x_j}\frac{\partial\mathcal{L}}{\partial(\partial_j u_i)}\right)\partial_l u_i \ , \tag{13.96}$$

we obtain

$$\frac{\delta\mathcal{L}}{\delta x_l} = \left[\frac{\partial\mathcal{L}}{\partial u_i} - \frac{\partial}{\partial x_j}\frac{\partial\mathcal{L}}{\partial(\partial_j u_i)}\right]\partial_l u_i + \frac{\partial}{\partial x_j}\left(\frac{\partial\mathcal{L}}{\partial(\partial_j u_i)}\partial_l u_i\right) + \left(\frac{\partial\mathcal{L}}{\partial x_l}\right)_{expl} . \tag{13.97}$$

The first term on the RHS is just the Euler-Lagrange equation, i.e. it vanishes, and noting that

$$\frac{\delta \mathcal{L}}{\delta x_l} = \frac{\partial \mathcal{L}}{\partial x_j} \delta_{lj} \ , \tag{13.98}$$

we finally obtain

$$\frac{\partial T_{lj}}{\partial x_j} = - \left(\frac{\partial \mathcal{L}}{\partial x_l} \right)_{expl} \ , \tag{13.99}$$

where $\boldsymbol{T}$ is the (elastic) energy-momentum tensor

$$T_{lj} \equiv -\mathcal{L}\delta_{lj} + \frac{\partial \mathcal{L}}{\partial(\partial_j u_i)} \partial_l u_i \ . \tag{13.100}$$

In the most general case, we have $\mathcal{L} = T - u$, where T is the kinetic energy density. Here, however, we did not consider $\partial_t u_i$ and hence do not include the kinetic energy. This implies $\mathcal{L} = -u$ and

$$T_{lj} = u\,\delta_{lj} - \frac{\partial u}{\partial(\partial_j u_i)} \partial_l u_i \ . \tag{13.101}$$

Surface integrals over $\boldsymbol{T}$, which enclose dissipative symmetry-breaking defects, define configurational forces

$$\mathcal{F}_l = \int_S T_{lj} \, dS_j \ , \tag{13.102}$$

that are thermodynamically conjugated to the defect coordinate ξ_l according to a dissipation inequality

$$\mathcal{F}_l \, \delta\xi_l \geq 0 \ . \tag{13.103}$$

XIV.   SUMMARY TABLE

Quantity	Notation
Reference/undeformed configuration	$\boldsymbol{X}$
Deformed configuration (spatial, Eulerian)	$\boldsymbol{x}$
The motion (mapping between $\boldsymbol{X}$ and $\boldsymbol{x}$)	$\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X})$
Displacement vector field	$\boldsymbol{U}(\boldsymbol{X},t) \equiv \boldsymbol{x}(\boldsymbol{X},t) - \boldsymbol{X} = \boldsymbol{x} - \boldsymbol{X}(\boldsymbol{x},t) = \boldsymbol{u}(\boldsymbol{x},t)$
Velocity vector field	$\boldsymbol{V}(\boldsymbol{X},t) \equiv \partial_t \boldsymbol{U}(\boldsymbol{X},t) = \boldsymbol{v}(\boldsymbol{x},t)$
Acceleration vector field	$\boldsymbol{A}(\boldsymbol{X},t) \equiv \partial_{tt} \boldsymbol{U}(\boldsymbol{X},t) = \boldsymbol{a}(\boldsymbol{x},t)$
Material derivative	$D_t \equiv \left(\frac{\partial}{\partial t}\right)_{\boldsymbol{X}} = \left(\frac{\partial}{\partial t}\right)_{\boldsymbol{x}} + \left(\frac{\partial}{\partial \boldsymbol{x}}\right)_t \left(\frac{\partial \boldsymbol{\varphi}(\boldsymbol{x},t)}{\partial t}\right)_{\boldsymbol{X}}$
Deformation gradient tensor	$\boldsymbol{F}(\boldsymbol{X},t) \equiv \nabla_{\boldsymbol{X}} \boldsymbol{\varphi}(\boldsymbol{X},t)$
Deformation gradient Jacobian (volume conversion)	$\boldsymbol{J}(\boldsymbol{X},t) \equiv \det \boldsymbol{F}(\boldsymbol{X},t)$
Surface element	$d\boldsymbol{S} = J^{-1} \boldsymbol{F}^T d\boldsymbol{s}$
Displacement gradient tensor	$\boldsymbol{H}(\boldsymbol{X},t) \equiv \nabla_{\boldsymbol{X}} \boldsymbol{U}(\boldsymbol{X},t),\ \boldsymbol{F} = \boldsymbol{I} + \boldsymbol{H}$
Biot extensional strain tensor	$\boldsymbol{E}_B \equiv \boldsymbol{U} - \boldsymbol{I}$
Hencky logarithmic strain tensor	$\boldsymbol{E_H} \equiv \ln \boldsymbol{U}$
Green-Lagrange strain tensor (Lagrangian)	$\boldsymbol{E} \equiv \frac{1}{2}\left(\boldsymbol{U}^2 - I\right) = \frac{1}{2}\left(\boldsymbol{H} + \boldsymbol{H}^T + \boldsymbol{H}^T \boldsymbol{H}\right)$
Euler-Almansi strain tensor (Eulerian)	$\boldsymbol{e} \equiv \frac{1}{2}\left(\boldsymbol{I} - \boldsymbol{F}^{-T} \boldsymbol{F}^{-1}\right)$
Linear (infinitesimal) strain tensor	$\boldsymbol{\varepsilon} \equiv \frac{1}{2}\left(\boldsymbol{H} + \boldsymbol{H}^T\right),\ \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$
Spatial velocity gradient tensor	$\boldsymbol{L} \equiv \frac{\partial \boldsymbol{v}(\boldsymbol{x},t)}{\partial \boldsymbol{x}} = \dot{\boldsymbol{F}} \boldsymbol{F}^{-1}$
Rate of deformation tensor	$\boldsymbol{D} \equiv \frac{1}{2}\left(\boldsymbol{L} + \boldsymbol{L}^T\right)$
Spin tensor (vorticity)	$\boldsymbol{W} \equiv \frac{1}{2}\left(\boldsymbol{L} - \boldsymbol{L}^T\right)$
Traction vector (deformed, reference)	$\boldsymbol{t}(\boldsymbol{x},t,\boldsymbol{n}),\ \ \boldsymbol{T}(\boldsymbol{X},t,\boldsymbol{N})$
Cauchy stress tensor	$\boldsymbol{\sigma}(\boldsymbol{x},t)$
Helmholtz free energy density	$f = u - Ts$
First Piola-Kirchhoff stress tensor	$\boldsymbol{P}(\boldsymbol{X},t) \equiv \frac{\partial f}{\partial \boldsymbol{F}(\boldsymbol{X},t)} = J\boldsymbol{\sigma} \boldsymbol{F}^{-T}$
Second Piola-Kirchhoff stress tensor	$\boldsymbol{S}(\boldsymbol{X},t) \equiv \frac{\partial f}{\partial \boldsymbol{E}(\boldsymbol{X},t)}$
Relation between stresses and tractions	$\boldsymbol{T}(\boldsymbol{X},t,\boldsymbol{N}) = \boldsymbol{P} \cdot \hat{\boldsymbol{N}} = \boldsymbol{\sigma} \cdot \hat{\boldsymbol{n}} = \boldsymbol{t}(\boldsymbol{x},t,\boldsymbol{n})$
Stiffness tensor (fourth order)	$\boldsymbol{C} \equiv \frac{\partial^2 u}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}},\qquad C_{ijkl} = \frac{\partial^2 u}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$

Elastic Moduli	Notation
Bulk Modulus	K
Young's Modulus	E
Lamé parameter	λ
Shear modulus	μ
Poisson's ratio	ν

Conservation laws	Mathematical formulation
General conservation form	$\frac{\partial(\text{field})}{\partial t} + \nabla_{\boldsymbol{x}} (\text{field flux}) = \text{source/sink}$
Mass conservation	$\partial_t \rho(\boldsymbol{x},t) + \nabla_{\boldsymbol{x}}(\rho(\boldsymbol{x},t)\boldsymbol{v}(\boldsymbol{x},t)) = 0$
Reynolds transport theorem	$\frac{D}{Dt}\int_\Omega \psi(\boldsymbol{x},t)\,d\boldsymbol{x}^3 = \int_\Omega [\partial_t \psi(\boldsymbol{x},t) + \nabla_{\boldsymbol{x}}(\psi(\boldsymbol{x},t)\boldsymbol{v}(\boldsymbol{x},t))]\,dx^3$
Linear momentum balance	$\boldsymbol{b} + \nabla_{\boldsymbol{x}} \cdot \boldsymbol{\sigma} = \rho\dot{\boldsymbol{v}}, \;\; \boldsymbol{B} + \nabla_{\boldsymbol{X}} \cdot \boldsymbol{P} = \rho_0\dot{\boldsymbol{V}}$
Angular momentum balance	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$

Thermodynamics	Mathematical formulation
First law	$\dot{\mathcal{K}} + \dot{\mathcal{U}} = \mathcal{P}_{ext} + \mathcal{Q}, \;\; \rho\dot{u} = \boldsymbol{\sigma}:\boldsymbol{D} - \nabla_{\boldsymbol{x}}\cdot\boldsymbol{q}$
Second law	$\dot{\mathcal{S}} \geq -\int_{\partial\Omega}\frac{\boldsymbol{q}\cdot\boldsymbol{n}}{T}ds + \int_\Omega \frac{r}{T}dx^3, \;\; \boldsymbol{\sigma}:\boldsymbol{D} - \rho\dot{f} - \rho s\dot{T} \geq 0$
Heat equation	$\rho\dot{u} = \boldsymbol{\sigma}:\boldsymbol{D} + \kappa\nabla_{\boldsymbol{x}}^2 T$

Linear elasticity	Mathematical formulation
Small deformation approximation	$|\boldsymbol{H}| \ll 1, \;\; \boldsymbol{E} \simeq \boldsymbol{\varepsilon} = \frac{1}{2}(\boldsymbol{H} + \boldsymbol{H}^T), \;\; \boldsymbol{D} \simeq \dot{\boldsymbol{\varepsilon}}$
Constitutive relation (general materials)	$\boldsymbol{\sigma} = \boldsymbol{C}:\boldsymbol{\varepsilon}$ ($\boldsymbol{C}$ contains 21 independent numbers)
Energy density (isotropic materials)	$u(\boldsymbol{\varepsilon}) = \frac{\lambda}{2}(tr\boldsymbol{\varepsilon})^2 + \mu tr\boldsymbol{\varepsilon}^2$
Hooke's law (isotropic materials)	$\boldsymbol{\sigma} = \lambda tr\boldsymbol{\varepsilon}I + 2\mu\boldsymbol{\varepsilon}, \; \sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}$
Navier-Lamé equation	$(\lambda + \mu)\nabla(\nabla \cdot \boldsymbol{u}) + \mu\nabla^2\boldsymbol{u} + \boldsymbol{b} = \rho\partial_{tt}\boldsymbol{u}$
Compatibility conditions (in 2D)	$\partial_{yy}\varepsilon_{xx} + \partial_{xx}\varepsilon_{yy} = 2\partial_{xy}\varepsilon_{xy}$
Airy stress function (in 2D)	$\nabla^2\nabla^2\chi = 0$
Helmholtz decomposition	$\boldsymbol{u} = \nabla\phi + \nabla \times \boldsymbol{\psi} \;\;\rightarrow\;\; c_d^2\nabla^2\phi = \partial_{tt}\phi, \;\; c_s^2\nabla^2\boldsymbol{\psi} = \partial_{tt}\boldsymbol{\psi}$
Wave speeds	$c_d = \sqrt{\frac{\lambda+2\mu}{\rho}}, \;\; c_s = \sqrt{\frac{\mu}{\rho}}$

Thermo-elasticity	Mathematical formulation
Free energy density	$f(\boldsymbol{\varepsilon},T) = \frac{1}{2}K(\mathrm{tr}\boldsymbol{\varepsilon})^2 + \mu(\varepsilon_{ij} - \frac{1}{3}\delta_{ij}\mathrm{tr}\boldsymbol{\varepsilon})^2 - K\alpha_T(T-T_0)\mathrm{tr}\boldsymbol{\varepsilon}$
Constitutive relation	$\sigma_{ij} = -K\alpha_T\left(T-T_0\right)\delta_{ij} + K\mathrm{tr}\boldsymbol{\varepsilon}\delta_{ij} + 2\mu(\varepsilon_{ij} - \frac{1}{3}\delta_{ij}\mathrm{tr}\boldsymbol{\varepsilon})$
Thermo-elastic Eqs. of motion (no inertia)	$(\lambda+\mu)\nabla\left(\nabla\cdot\boldsymbol{u}\right) + \mu\nabla^2\boldsymbol{u} = \alpha_T K\nabla T$

Nonlinear elasticity	Mathematical formulation
Free energy density (per unit volume in the reference config.)	$f(\boldsymbol{E},T) = u(\boldsymbol{E},T) - Ts(\boldsymbol{E},T)$
Incompressible neo-Hookean material	$u = \frac{1}{2}\mu[\mathrm{tr}(\boldsymbol{F}^T\boldsymbol{F}) - 3] - \alpha(J-1)$
Saint-Venant material	$u = \frac{\lambda}{2}\mathrm{tr}^2\boldsymbol{E} + \mu\,\mathrm{tr}\boldsymbol{E}^2$

Linear visco-elasticity	Mathematical formulation
Newtonian (linear) viscosity	$\eta = \lim\limits_{\dot{\varepsilon}\to 0} \sigma/\dot{\varepsilon}$
Constitutive relation (with stress relaxation modulus)	$\sigma_{ij}\left(t\right) = \int_{-\infty}^{t} G_{ijkl}\left(t-t'\right)\dot{\varepsilon}_{kl}\left(t'\right)dt'$
Constitutive relation (with creep compliance modulus)	$\varepsilon_{ij}\left(t\right) = \int_{-\infty}^{t} J_{ijkl}\left(t-t'\right)\dot{\sigma}_{kl}\left(t'\right)dt'$
Kelvin-Voigt model	$\sigma = \sigma^{vis} + \sigma^{el}$ (and the same strain)
Maxwell model	$\dot{\varepsilon} = \dot{\varepsilon}^{el} + \dot{\varepsilon}^{vis}$ (and the same stress)

Plasticity	Mathematical formulation
Ideal elasto-(perfect)plasticity	$\sigma = E\varepsilon$ for $E\varepsilon < \sigma_y$ and $\sigma = \sigma_y$ for $E\varepsilon \geq \sigma_y$
vom Mises criterion	$\sqrt{\dfrac{(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_1-\sigma_3)^2}{6}} = \sigma_y$
Tresca criterion	$\frac{1}{2}\max\left(\left.\left|\sigma_i - \sigma_j\right|\right|_{i\neq j}\right) = \sigma_y$
Contour integral around a topological defect	$\oint d\boldsymbol{u} = \boldsymbol{b}$
Hyper-elastoplasticity	$\boldsymbol{F} = \boldsymbol{F}^{el}\boldsymbol{F}^{pl}$
Hypo-elastoplasticity	$\boldsymbol{D} = \boldsymbol{D}^{el} + \boldsymbol{D}^{pl}$