Concepts of condensed matter physics

Spring 2021

Exercise #3

Due date: 23/06/2021

1. **Symmetry and Goldstone.** Consider the following action (consult "Quantum Field Theory of Many-Body Systems" by Xiao-Gang Wen; pages 82-83)

$$S = \int_0^\beta d\tau \int d^d x \psi^* \left(\partial_\tau - \frac{\nabla^2}{2m} + \alpha + \beta|\psi|^2\right)\psi$$

   a. Write the complex field ψ in a polar representation, i.e. $\psi = \sqrt{\rho}e^{i\theta}$. What is the mean-field value of ρ?

   b. Show that the action has a global $U(1)$ symmetry of the form$\theta \rightarrow \theta + const.$

   c. Since the above is a continuous symmetry there must be a Goldstone mode associated with it. By integrating out the massive Gaussian fluctuations $\delta\rho$ of the superfluid density ρ around the mean field value $\langle\rho\rangle$, show that the action of this Goldstone assumes the form

$$S_{XY} = -\int_0^\beta d\tau \int d^d x \theta(\chi\partial_\tau^2 + \rho_s \nabla^2)\theta$$

   This action is similar to that of the classical XY-model (in the continuum limit), and describes the low energy excitations of a superfluid. (Here ρ_s and χ are known as the *superfluid stiffness* and *compressibility*)

   d. What is the action you would get if you were to neglect the fluctuations $\delta\rho$ of the superfluid density ρ altogether?

   e. Return to the effective XY model describing the Goldstone modes. Define an appropriate correlation function that distinguishes between an ordered and a disordered phase, and calculate its long-range behavior (like we did in the tutorial) for the d=1, 2, 3 cases at zero temperature. Discuss the difference between the different dimensions.

   f. We know that S has vortex excitations in d=1 at zero temperatures and in d=2 at finite temperatures. Write a typical vortex configuration for each of these cases. What is the action associated with a vortex? Thinking of vortices as thermal excitations, which excitation is more probable? (i) Two single vortices or (ii) one double vortex (winding number = 2)? Explain.

2. **Debye-Waller factor of low dimensional crystals and the Mermin-Wagner theorem** (Consult the L and N appendices of "Solid State Physics" By Neil Ashcroft and David Mermin). In this question we will show that in low dimensional systems the fluctuations associated with the Goldstone modes of a crystal (a.k.a. phonons) diverge and destroy the long range order even if they are small on the microscopic scale. To see that, we will perform a full quantum mechanical treatment of the problem. Like we did in class, we will first assume that the fluctuations are small. This will allow us to derive an effective theory. Using this theory we will find that in low dimensions the fluctuations can actually be very large when we look at large distances, in conflict with the original assumption.

To be specific, we consider the Hamiltonian of ions in a cubic crystal phase of general dimension d

$$H = \sum_{j=1}^{N} \frac{\boldsymbol{P}_j^2}{2M} + \sum_{\langle ij \rangle} V(\boldsymbol{r}_i - \boldsymbol{r}_j)$$

The $\langle ij \rangle$ brackets denote summation over nearest neighbors.

Let us denote the classical ground state positions of the ions by $\{\boldsymbol{R}_j\}_{j=1}^{N}$. We can expand the potential $V(\boldsymbol{r})$ up to quadratic order in deviations around the ions' classical ground state positions, i.e. we take $\boldsymbol{r}_j = \boldsymbol{R}_j + \boldsymbol{u}_j$ where $\langle |\boldsymbol{u}_j| \rangle \ll a$, and a is the inter-ion distance. A typical low-energy Hamiltonian then assumes the form

$$H = \sum_{i} \frac{\boldsymbol{P}_i^2}{2M} + \sum_{\langle ij \rangle} \frac{K}{2} (\boldsymbol{u}_i - \boldsymbol{u}_j)^2 .$$

This is nothing but an array of coupled harmonic oscillators.

a. Diagonalize the Hamiltonian using the ladder operators in quasi-momentum space, a_k, such that it takes the simple form $H = \sum_k \omega_k \left(a_k^{+} a_k + \frac{1}{2} \right)$. Plot the Goldstone mode dispersion within the first Brillouin zone.

<u>Comment:</u> To understand if the system maintains long-range order (LRO) we consider the density-density correlation function, given by

$$C(\boldsymbol{r}, \boldsymbol{r}'; t, t') \equiv \langle \rho(\boldsymbol{r}, t) \rho(\boldsymbol{r}', t') \rangle$$

where $\langle O \rangle = \frac{Tr[e^{-\beta H} O]}{Tr e^{-\beta H}}$ denotes quantum averaging in a thermal ensemble, such that $\langle a_k^{+} a_k \rangle = \frac{1}{e^{\beta \omega_k - 1}}$. Here the density operator is defined as follows

$$\rho(\boldsymbol{r}, t) \equiv \sum_{j=1}^{N} \delta\left(\boldsymbol{r} - \boldsymbol{r}_j(t) \right)$$

If LRO exists throughout the system we expect that in the limit $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$ the function $C(\boldsymbol{r}, \boldsymbol{r}'; 0,0)$ will have a finite amplitude modulation at the crystal periodicity. The physics behind this notion is rigidity, namely, if we perturb an ion at $\boldsymbol{r}$ then the ion at $\boldsymbol{r}'$ will move in correlation with its motion (even if $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$).

b. Use the space and time translational invariance of the correlation function (i.e. $C(\boldsymbol{r},\boldsymbol{r}';t,t') = C(\boldsymbol{r}-\boldsymbol{r}';t-t')$)) to show that it's Fourier transform is given by

$$C(\boldsymbol{q},\boldsymbol{k};\omega,\omega') = V\delta_{\boldsymbol{k},\boldsymbol{q}}(2\pi)\delta(\omega+\omega')S(\boldsymbol{q},\omega),$$

where the Fourier transform is defined as

$$C(\boldsymbol{q},\boldsymbol{k};\omega,\omega') = \int d^d r d^d r' dt dt' C(\boldsymbol{r},\boldsymbol{r}';t,t') e^{i(\boldsymbol{q}\cdot\boldsymbol{r}+\boldsymbol{k}\cdot\boldsymbol{r}'+\omega t+\omega' t')}$$

and

$$S(\boldsymbol{q},\omega) = \frac{1}{V}\sum_{jj'}\int dt e^{-i\omega t}\langle e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_j(t)} e^{i\boldsymbol{q}\cdot\boldsymbol{r}_{j'}(0)}\rangle$$

Note that this function is known as the *dynamic structure factor*. Do not forget that we are working in a finite size system where $V = Na^d$.

c. Use the identity $\langle e^{A+B}\rangle = e^{1/2\langle (A+B)^2\rangle}$ to show that you can write the dynamic structure factor $S(q,\omega)$ in the form

$$S(q,\omega) = \frac{e^{-2W}}{a^d}\sum_{j=1}^{N} e^{iq\cdot R_j}\int dt e^{-i\omega t}\, e^{\langle (q\cdot u_0)(q\cdot u_j(t))\rangle}$$

where $W \equiv \frac{1}{2}\langle (q\cdot u_0)^2\rangle$ is known as the *Debye-Waller* factor.

d. Compute the Debye-Waller factor for a general dimension d. For simplicity assume that the phonons have a linear dispersion, which is cutoff by the Debye frequency ω_D set by the width of the dispersion band.

<u>Comment:</u> To obtain the long range modulations we take the term in the exponent to be unity such that the sum over j can be performed (the idea is that delta functions in q-space translate to pure long-range modulations in real space). In such a case one would obtain

$$S(q,\omega) \propto e^{-2W}\sum_G \delta_{qG}$$

where G are the reciprocal lattice vectors. This result implies that for very low frequencies the delta functions are weighted by Ne^{-2W}.

e. Show that in one dimension W diverges for all temperatures. Is zero temperature different?

f. Show that in two-dimensions W diverges at finite temperatures.

g. Show the similarity between the one-dimensional case at zero temperature and the two-dimensional case at finite temperatures. Can you explain this in terms of path integrals?

3. Spin-wave dispersion (Consult "Interacting Electrons and Quantum Magnetism" by A. Auerbach pages 123 - 126).

In this question you are asked to derive the spin-wave dispersion of the two-dimensional Heisenberg model on a square lattice with antiferromagnetic coupling (i.e., $J > 0$). The Hamiltonian of such a model is given by

$$H = J \sum_{\langle ij \rangle} \left[S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right]$$

where $S^+ = (S^x + S^y)/2$ and $S^- = (S^+)^+$ are the spin raising and lowering operators, and $S^{x,y,z}$ are the spin-half operators which are arranged on a square lattice. The $\langle ij \rangle$ brackets denote summation over nearest neighbors.

a. Separate the lattice into two sub-lattices, A and B, such that all the neighbors of an A site are B's and vice versa. Now take $\langle S_j^z \rangle = \eta(j)$ where $\eta(j) = 1$ if $j \in A$ and $\eta(j) = -1$ if $j \in B$. What is the ground state-energy given by this solution?

b. Show that the mean-field solution you have obtained is not an eigenstate of the Hamiltonian, and thus is not the true ground state.

c. Now let us refine the solution by accounting for quantum fluctuations. First apply a rotation of π about the x axis to all spins on sub-lattice B $\boldsymbol{S}_j \to \tilde{\boldsymbol{S}}_j$ (the idea is that we expand the Hamiltonian around the mean-field solution, where we have assumed that the spins are aligned along the z direction and anti-parallel to all their nearest neighbors). Now let us assume that all spins are fluctuating weakly around $\langle \tilde{S}_i^z \rangle \approx \frac{1}{2}$, such that we may introduce the Holstein-Primakoff bosons

$$S^z = \frac{1}{2} - n_b$$

$$S^+ = \sqrt{1 - n_b}\, b$$

$$S^- = b^+ \sqrt{1 - n_b}$$

where $n_b = b^+ b$. Apply this transformation

d. Diagonalize the Bosonic theory using a Bogoliubov transformation. Plot the spin-wave dispersion schematically. (Note that in the limit of weak fluctuations $\langle n_b \rangle \ll 1$.)

e. In class you have derived the spin-dispersion of the ferromagnetic model (i.e., $J < 0$). Discuss the difference in the long wave-length dependence.