Concepts of condensed matter physics

Spring 2013

Exercise #3

Due date: 1/05/2013

1. **Debye-Waller factor of low dimensional crystals and the Mermin-Wagner-Berezinskii theorem** (I strongly encourage you to 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 of a Goldstone mode can diverge and destroy the long range order even if they are small on the microscopic scale. We will do this by first assuming that the fluctuations are small which will allow us to derive an effective theory. Using this theory we will find that the fluctuations are actually very large in conflict with the original assumption.

   a. Consider the Hamiltonian of ions in a cubic crystal phase

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

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

   Let us denote the classical ground state positions of the ions by $\{\boldsymbol{R}_j\}_{j=1}^{N}$.

   Now we expand the potential $V(\boldsymbol{x})$ up to quadratic order in deviations around their classical ground state position, i.e. we take $\boldsymbol{r}_j = \boldsymbol{R}_j + \boldsymbol{u}_j$ where $\langle |\boldsymbol{u}_j| \rangle \ll a$ and a being the inter-ion distance. The Hamiltonian then assumes the form

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

   which is nothing but an array of coupled harmonic oscillators.

   Diagonlaize the Hamiltonian using the ladder operators in quasimomentum space, a_k, such that it takes the simple form $H = \sum_k \omega_k \left(a_k^+ a_k + \frac{1}{2}\right)$. Draw the Goldstone mode dispersion.

b. 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 $\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta H} O\right]}{\mathrm{Tr} e^{-\beta H}}$ 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

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

If LRO exists throughout the system we expect that this function will modulate with crystal precocity infinitely far away. The physics behind this notion is rigidity, namely, if we perturb an ion at $\boldsymbol{r}$ then the ion at $\boldsymbol{r}'$is correlated with its motion even if $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$.

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

$$S(\boldsymbol{q}, \omega) = \frac{1}{N^2} \sum_{jj'} \int_0^\infty \frac{dt}{2\pi}\, e^{i\omega t} \langle e^{i\, \boldsymbol{q}\, r_j} e^{-i\, \boldsymbol{q}\, r_{j'}} \rangle$$

Note that this function is known as the dynamic structure factor.

c. Before we continue we will need to use the identity

$$\langle e^A e^B \rangle = e^{\langle A^2 + 2\, A\, B + B^2 \rangle / 2}$$

where A and B are linear functions of a and a^+. Bonus: prove this identity following the short article by David Mermin, Journal of Mathematical Physics, **7**, 1038 (1966).

- Use the Baker-Campbell-Hausdoerff formula to show that

$$\langle e^{\sum_k (c_k a_k + d_k a_k^+)} \rangle = \langle e^{\sum_k c_k a_k} e^{\sum_k d_k a_k^+} \rangle e^{-\frac{1}{2} \sum_k c_k d_k}$$

where $c_k$and d_k are some momentum dependent pre-factors, such they are c-numbers

- Insert the unity operator $1 = e^{-\beta H} e^{\beta H}$ and use the cyclic property of the trace to show that
$\langle e^{\sum_k c_k a_k} e^{\sum_k d_k a_k^+} \rangle = e^{\sum_k c_k d_k} \langle e^{\sum_k (e^{-\beta\omega_k} c_k a_k)} e^{\sum_k d_k a_k^+} \rangle$
- Iterate this relation an infinite amount of times to show that

$$\langle e^{\sum_k c_k a_k} e^{\sum_k d_k a_k^+} \rangle = e^{\sum_k \frac{c_k d_k}{1-e^{-\beta\omega_k}}} \langle e^{\sum_k d_k a_k^+} \rangle$$

Since $\langle e^{\sum_k d_k a_k^+} \rangle = 1$ we have shown that

$$\langle e^{\sum_k c_k a_k} e^{\sum_k d_k a_k^+} \rangle = e^{\sum_k \frac{c_k d_k}{1-e^{-\beta\omega_k}}}$$

and thus

$$\langle e^{\sum_k (c_k a_k + d_k a_k^+)} \rangle = e^{\frac{1}{2}\sum_k c_k d_k \coth\frac{\beta\omega_k}{2}}$$

- Now to complete the job compute
$e^{-\frac{1}{2}\langle (\sum_k (c_k a_k + d_k a_k^+))^2 \rangle}$ to show that it gives the same result.

d. Use the identity above, and, again the invariance of space and time to show that you can write the dynamic structure factor $S(\boldsymbol{q}, \omega)$ in the following manner

$$S(\boldsymbol{q}, \omega) = \frac{e^{-2W}}{N} \sum_{j=1}^{N} e^{i\boldsymbol{q}\cdot\boldsymbol{R}_j} \int_0^\infty \frac{dt}{2\pi} e^{i\omega t} e^{\langle (\boldsymbol{q}\cdot\boldsymbol{u}_0) (\boldsymbol{q}\cdot\boldsymbol{u}_j(t)) \rangle}$$

where $W \equiv \frac{1}{2}\langle (\boldsymbol{q}\cdot\boldsymbol{u}_0)^2 \rangle$ is the *Debye-Waller* factor.

e. Compute the Debye-Waller factor for a general dimension d. Here you may assume that the phonons have a linear dispersion, which is cutoff by the Debye frequency ω_D. To obtain the long range modulations we take the term in the exponent (within the sum) 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

$$S(\boldsymbol{q}, \omega) \approx Ne^{-2W} \delta_{\boldsymbol{qG}}$$

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

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

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

h. Do you identify any 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?

i. In class you have seen the example of a ferromagnet where spin is conserved, and thus the dispersion is quadratic. How would your results change for a quadratic Goldstone mode?

2. **Spin-wave dispersion** (Please, by all means 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. 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 $J > 0$. $S^+ = (S^x + S^y)/2$ 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. Obtain the mean-field ground state solution. First, 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 $\langle S_j^z \rangle = (-1)^{\eta(j)}$ 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 eigen-state 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 $\boldsymbol{S}_j \rightarrow \tilde{\boldsymbol{S}}_j$ (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 $\langle \tilde{S}_i^z \rangle \approx 1$, such that we may introduce the Holstein-Primakoff bosons

$$S^z = 1 - n_b$$
$$S^+ = \sqrt{2 - n_b}\, b$$
$$S^- = b^+ \sqrt{2 - n_b}$$

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?