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PHYS 7450: Advanced Solid State Physics

Homework Set 2

Issued January 27, 2015
Due February 10, 2015

Reading Assignment: My lecture notes and J. Solyom, Solids 1, Ch. 11, 12, 13

1. Coordinate to Fourier space transformation

   Use the Fourier integral transform $\phi(\mathbf{r}) = \int \frac{d^dk}{(2\pi)^d} e^{i\mathbf{k}\cdot\mathbf{r}} \tilde{\phi}(\mathbf{k})$ to demonstrate a very important result

$$
\begin{aligned}
H &= \frac{1}{2}\int d^drd^dr'\phi(\mathbf{r})\Gamma(\mathbf{r}-\mathbf{r}')\phi(\mathbf{r}'), \\
&= \frac{1}{2}\int \frac{d^dk}{(2\pi)^d}\tilde{\phi}(-\mathbf{k})\tilde{\Gamma}(\mathbf{k})\tilde{\phi}(\mathbf{k}), \qquad (1)
\end{aligned}
$$

   for converting a Hamiltonian from real-space $\phi(\mathbf{r})$ to Fourier $\tilde{\phi}(\mathbf{k})$ degrees of freedom is, that we will use repeatedly throughout the course.

2. Quantum phonon correlators

   Consider a general quantum model (with a single atom per unit cell for simplicity) of a three dimensional harmonic crystal defined by natural frequencies $\omega_{\mathbf{k},i}$ (i labels the three band corresponding to three dimensions) described by the Hamiltonian

$$
\begin{aligned}
H_{ph} &= \sum_{\mathbf{k}\in 1BZ}\left[\frac{1}{2M}\tilde{\mathbf{P}}^\dagger_{\mathbf{k}}\cdot\tilde{\mathbf{P}}_{\mathbf{k}} + \frac{1}{2}\tilde{\mathbf{u}}^\dagger_k\cdot\mathbf{D}_{\mathbf{k}}\cdot\tilde{\mathbf{u}}_k\right], \qquad (2) \\
&= \sum_{i,\mathbf{k}\in 1BZ}\left[\frac{1}{2M}\tilde{P}^\dagger_{\mathbf{k},i}\tilde{P}_{\mathbf{k},i} + \frac{1}{2}M\omega^2_{\mathbf{k},i}\tilde{u}^\dagger_{\mathbf{k},i}\tilde{u}_{\mathbf{k},i}\right], \qquad (3)
\end{aligned}
$$

   discussed in class.

   Using the representation of the phonon field $\mathbf{u_R}$ in terms of the normal modes and the corresponding creation and annihilation operators, $a^\dagger_{\mathbf{k},i}, a_{\mathbf{k},i}$

(a) Show that phonon correlation function at finite temperature is given by

$$\langle \mathbf{u_R} \cdot \mathbf{u_{R'}} \rangle = \frac{1}{2N} \sum_{i,\mathbf{k} \in 1BZ} \frac{\hbar}{M\omega_{\mathbf{k},i}} \coth(\frac{\hbar\omega_{\mathbf{k},i}}{2k_B T}) e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R'})}, \tag{4}$$

where we used the normal modes finite-T Bose-Einstein occupation $N_{\mathbf{k}}$ derived for bosons.

(b) Use above result to show that mean-squared phonon fluctuations, $u_{rms}^2 = \langle \mathbf{u_R} \cdot \mathbf{u_R} \rangle$,

i. In the $T = 0$ ($k_B T \ll \hbar\omega_D$), quantum limit are given by

$$u_{rms}^2 = \frac{1}{2N} \sum_{i,\mathbf{k} \in 1BZ} \frac{\hbar}{M\omega_{\mathbf{k},i}},$$

and that for 3d degenerate acoustic Debye phonons ($\omega_{\mathbf{k},i} = c_s k$) reduce to

$$u_{rms}^2 = \frac{3}{16} \frac{\hbar a}{M c_s} \approx \frac{\hbar}{M\omega_D}, \tag{5}$$

$$\tag{6}$$

in the continuum limit of $N = L^3/a^3 >> 1$ (a is a lattice constant). Note the units are correct length-squared.

ii. In the high T ($k_B T \gg \hbar\omega_D$), classical limit are given by

$$u_{rms}^2 = \frac{1}{N} \sum_{i,\mathbf{k} \in 1BZ} \frac{k_B T}{M\omega_{\mathbf{k},i}^2},$$

and that for 3d degenerate acoustic Debye phonons ($\omega_{\mathbf{k},i} = c_s k$) reduce to

$$u_{rms}^2 = 3\frac{k_B T}{2M c_s^2} a^2 \approx \frac{k_B T}{\hbar\omega_D} a^2, \tag{7}$$

in the continuum limit of $N = L^3/a^3 >> 1$ (a is a lattice constant). Note: (i) the units are correct length-squared, (ii) the equipartion is recovered as expected for a harmonic oscillator in this limit.

Hints:

- Continuum limit allows you to replace the sum over $\mathbf{k}$ by an integral according to $\sum_{\mathbf{k}} \ldots \to L^3 \int \frac{d^3k}{(2\pi)^3} \ldots$.
- Introduce a short scale (ultra-violet) cutoff on the largest frequency ω_D, corresponding to the largest momentum $\Lambda = \pi/a$.
- Do not worry about factors of order 1, as above is just an estimate, with the quantitatively accurate answer (that you are not asked to produce) requiring careful treatment of the actual phonon dispersion rather than just using the Debye model.

(c) Using Lindemann criterion together with result (b) ii, roughly, what is the melting temperature T_m of for a typical crystal in terms of its Debye frequency?

(d) Repeat your calculation in (b) ii for two dimensions (2d) and show that it is now given by

$$u^2_{rms,2d} = \frac{k_B T}{\pi M c_s^2}\, a^2 \ln(L/a),$$

fluctuations that diverge logarithmically with the growing system size $L/a \to \infty$. What do you think the qualitative consequence of this result for 2d crystals? This divergence is a manifestation of the so-called Hohenberg-Mermin-Wagner theorem, that in particle physics is referred to as the Coleman's theorem.

Hint: In addition to the uv (short-scale) cutoff, here you will need to also introduce an infrared (long scale) cutoff as the size of the sample L, limiting the wavevectors to $k > \pi/L$.

(e) Use above analyses for a harmonic phonon field to show that the static structure function

$$S(\mathbf{q}) \;=\; \frac{1}{N}\sum_{\mathbf{R},\mathbf{R}'} e^{-i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')}\langle e^{-i\mathbf{q}\cdot\mathbf{u}_{\mathbf{R}}} e^{i\mathbf{q}\cdot\mathbf{u}_{\mathbf{R}'}}\rangle, \tag{8}$$

is given by

$$S(\mathbf{q}) \;=\; \frac{1}{N}\sum_{\mathbf{R},\mathbf{R}'} e^{-i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} e^{-C_{\mathbf{R}-\mathbf{R}'}}, \tag{9}$$

with the equal-time correlator

$$C_{\mathbf{R}-\mathbf{R}'} \;=\; \frac{1}{2N}\sum_{i,\mathbf{k}\in 1BZ} \frac{\hbar}{M\omega_{i,\mathbf{k}}}(\mathbf{q}\cdot\hat{\mathbf{e}}_{\mathbf{k},i})^2 \coth\left(\frac{\hbar\omega_{\mathbf{k},i}}{2k_B T}\right)\left(1 - e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{R}')}\right). \tag{10}$$

Hint:

Use a very useful identity, valid for quadratic (Gaussian) operator fields

$$\langle e^A e^B\rangle = e^{\frac{1}{2}\langle A^2\rangle + \frac{1}{2}\langle B^2\rangle + \langle AB\rangle}, \tag{11}$$

that can be derived by using Baker-Hausdorff formula (valid for operators whose commutator is a c-number)

$$e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]} \tag{12}$$

together with a formula

$$\langle e^{\phi}\rangle = e^{\frac{1}{2}\langle \phi^2\rangle},$$

that we have derived for classical harmonic (Gaussian) fields using Gaussian integrals, but can also be shown to hold for quantum harmonic fields using path-integral formulation.

(f) Evaluate above correlator $C_{\mathbf{R}-\mathbf{R}'}$ in the continuum classical limit, for simplicity specializing to an isotropic crystal with $\lambda = -\mu$, with linear dispersion (Debye model) showing that at long scales it behaves according to

$$C_{\mathbf{R}-\mathbf{R}'} \approx \eta_q(T) \ln\left(|\mathbf{R}-\mathbf{R}'|/a\right). \tag{13}$$

Find the exponent $\eta_q(T)$.

Hint:

This is an asymptotic long scale result. You will need to introduce a short-scale uv cutoff $\Lambda = \pi/a$. Don't worry too much about factors of order one, particularly when they appear inside the argument of a logarithm, where they are harmless.

(g) Use above results to demonstrate that at finite temperature T, a structure function of a 2D crystal no longer exhibits true (δ-function) Bragg peaks, but instead is characterized by *quasi*-Bragg power-law peaks

$$S(\mathbf{q}) \sim v \sum_{\mathbf{G}_p} \frac{1}{|\mathbf{q}-\mathbf{G}|^{2-\eta_q}}, \tag{14}$$

i.e., translatonal *quasi*-long-range order, with reciprocal lattice $\mathbf{G}$.

Hint:

To evaluate the sum over $\mathbf{R}$, use the Poisson summation formula

$$\sum_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} = \sum_{\mathbf{G}} (2\pi)^d \delta^d(\mathbf{q}-\mathbf{G}),$$

where $\mathbf{G}$ span a reciprocal lattice to the real-space lattice of $\mathbf{R}$.

3. Nonlinear elasticity and thermal expansion

Consider a real crystal that exhibit nonlinear elasticity, with elastic energy still given quadratically in the elastic strain $u_{\alpha\beta}$

$$H_{el}[\mathbf{u}(\mathbf{r})] = \frac{1}{2}\int d^d r C_{\alpha\beta,\gamma\delta}\, u_{\alpha\beta} u_{\gamma\delta}, \tag{15}$$

however with strain a nonlinear function of the phonon field $\mathbf{u}$.

(a) Using a distorted atomic position $\mathbf{R}(\mathbf{r}) = \mathbf{r} + \mathbf{u}(\mathbf{r})$ labelled by a local relaxed position $\mathbf{r}$ and the definition of the nonlinear strain in terms of the metric tensor

$$u_{\alpha\beta} = \frac{1}{2}(g_{\alpha\beta} - \delta_{\alpha\beta}) = \frac{1}{2}(\partial_\alpha \mathbf{R}\cdot\partial_\beta \mathbf{R} - \delta_{\alpha\beta}) \tag{16}$$

show that the nonlinear strain is given exactly by

$$u_{\alpha\beta} = \frac{1}{2}(\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha \mathbf{u}\cdot\partial_\beta \mathbf{u}). \tag{17}$$

(b) Using above result and the elastic Hamiltonian, (15), above, show that the nonlinear part of the elastic Hamiltonian density $\mathcal{H}_{el} = \mathcal{H}_{0,el} + \mathcal{H}_{nonlin}$ is given by

$$\begin{aligned}\mathcal{H}_{nonlin} &= \mu(\partial_\alpha u_\beta)(\partial_\alpha \mathbf{u}\cdot\partial_\beta \mathbf{u}) + \frac{\lambda}{2}(\partial_\alpha u_\alpha)(\partial_\beta \mathbf{u}\cdot\partial_\beta \mathbf{u}) \\ &+ \frac{\mu}{4}(\partial_\alpha \mathbf{u}\cdot\partial_\beta \mathbf{u})(\partial_\alpha \mathbf{u}\cdot\partial_\beta \mathbf{u}) + \frac{\lambda}{8}(\partial_\alpha \mathbf{u}\cdot\partial_\alpha \mathbf{u})(\partial_\beta \mathbf{u}\cdot\partial_\beta \mathbf{u}), \end{aligned} \quad (18)$$

with cubic and quartic nonlinearities, and $\mathcal{H}^0_{el}$ the harmonic energy density, (3).

(c) As discussed in class (see lecture notes) for low T, but still in the classical limit ($k_B T \gg \hbar\omega_k$) phonon fluctuations are small and can be treated using classical statistical mechanics. By Taylor-expanding in the small strain $\partial_\alpha u_\beta$ in above nonlinearities and in δV, derive (but do not actually calculate) the formal expression (in terms of integrals over products of phonon correlators $G_{\alpha\beta}(\mathbf{r}) = \langle u_\alpha(\mathbf{r}) u_\beta(\mathbf{0})\rangle_0$) for the *lowest* order contributions to the change in the volume of the sample

$$\delta V = \langle \int d^d r (\sqrt{\det \mathbf{g}} - 1)\rangle. \quad (19)$$

Please note that some terms seemingly contributing to δV actually vanish in the averaging process due to symmetry. Thus, those vanishing terms do not count as the "lowest order". Thus I am asking you to derive the contribution to δV from the lowest *nonvanishing* terms.

4. Quantization of a bosonic Hamiltonian

In this problem you will second-quantize the Schödinger equation, in preparation of our study of weakly interacting superfluids, as for example an atomic gas of degenerate Rb^{85} as studied in JILA.

(a) Let us begin with a noninteracting action

$$S_0 = \int dt d^3 r \left(i\hbar \psi^\dagger \frac{\partial \psi}{\partial t} + \psi^\dagger \frac{\hbar^2}{2m}\nabla^2 \psi \right)$$

for a bosonic field $\psi(\mathbf{r})$. By writing down a functional version of the Euler-Lagrange equation, $\frac{\delta S}{\delta \psi^\dagger(\mathbf{r})} = 0$, show that it gives a Schrödinger equation, but now understood as a wave equation for a field $\psi(\mathbf{r})$ (analog of our phonon equation for sound $\mathbf{u}(\mathbf{r})$ or the Maxwell's wave equation for an electromagnetic field, $\mathbf{E}(\mathbf{r})$).

(b) Repeat this derivation from the Hamiltonian approach:

i. find the momentum conjugate to $\psi(\mathbf{r})$ using standard definition of a conjugate momentum from Lagrangian formulation of mechanics,

ii. write down the canonical commutation relations,

iii. write down the Hamiltonian, and the corresponding equations of motion.

(c) Using the normal-modes expansion, $\psi(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$ write down the Hamiltonian in terms of the decoupled normal modes $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^{\dagger}$ and derive their commutation relation from the canonical one for $\psi(\mathbf{r})$ and $\Pi(\mathbf{r})$.

(d) Using a more convenient normal mode expansion for dynamic Heisenberg field $\psi(\mathbf{r}, t) = \int \frac{d\omega d^d k}{(2\pi)^{d+1}} \tilde{\psi}(\mathbf{k}, \omega) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t}$ express the action in terms of these modes, $\psi(\mathbf{k}, \omega)$.

(e) Use grand-canonical quantum statistical mechanics for these conserved bosons (by using chemical potential μ to control the atom number) to express the average of number operator $\hat{N} = \int_{\mathbf{r}} \psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})$,

$$N(\mu) = \frac{1}{Z}\mathrm{Tr}\left[\hat{N} e^{-\beta(H_0 - \mu\hat{N})}\right] \tag{20}$$

in terms of the chemical potential, μ. Note that the answer has the same form as that for phonons, except the dispersion is nonrelativistic here and the chemical potential is finite, as (in contrast to phonon number) atoms are conserved.