Homework 2, 620 Many body

October 26, 2023

1) Problem 4.5.5 in A&S: Using the frequency summation technique compute the following correlation functions:

$$\chi^s(\mathbf{q}, i\Omega) \;=\; -\frac{1}{\beta} \sum_{\mathbf{p}, i\omega_n} G^0(\mathbf{p}, i\omega_n) G^0(-\mathbf{p} + \mathbf{q}, -i\omega_n + i\Omega) \tag{1}$$

$$\chi^c(\mathbf{q}, i\Omega) \;=\; -\frac{1}{\beta} \sum_{\mathbf{p}, i\omega_n} G^0(\mathbf{p}, i\omega_n) G^0(\mathbf{p} + \mathbf{q}, i\omega_n + i\Omega) \tag{2}$$

where

$$G^0(\mathbf{q}, i\omega_n) = \frac{1}{i\omega_n - \varepsilon_p} \tag{3}$$

and $i\Omega$, $i\omega_n$ are bosonic, fermionic Matsubara frequencies, respectively.

2) Problem 4.5.6 in A&S: Pauli paramagnetic susceptibility occurs due to the coupling of the magnetic field to the spin of the conduction electrons. The corresponding Hamiltonian is:

$$H = H^0[c^\dagger, c] - \mu_0 \vec{B} \sum_{\mathbf{k},s,s'} c^\dagger_{\mathbf{k},s} \vec{\sigma}_{s,s'} c_{\mathbf{k},s'} \tag{4}$$

where H^0 is the non-interacting electron Hamiltonian with dispersion ε_k.

Calculate the free energy of the system (in the presence of the magnetic field) and show that the magnetic susceptibility ($\chi = \partial^2 F/\partial B^2$ at $B = 0$) at low temperature is $\frac{\mu_0}{2}\rho(E_F)$, where $\rho(E_F)$ is the density of electronic states at the Fermi level.

3) Problem 4.5.7 in A& S: Electron-phonon coupling.

In the first few lectures we showed how we can obtain the phonon dispersion in a material. The quantum solution in terms of independent harmonic oscillators has the usual form

$$H_{ph} = \sum_{\mathbf{q},\nu} \omega_{\mathbf{q},\nu}\, a^\dagger_{\mathbf{q},\nu} a_{\mathbf{q},\nu} \tag{5}$$

where $\mathbf{q}$ is momentum in the 1BZ, and ν is a phonon branch. The Fourier transform of the oscillation amplitude is

$$u^\nu_{\mathbf{q},\alpha,j} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_n} u^\nu_{n,\alpha,j} e^{-i\mathbf{q}\mathbf{R}_n} \tag{6}$$

Here α is the Wickoff position in the unit cell, j is x, y, z and $\mathbf{R}_n$ is the lattice vector to unit cell at $\mathbf{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$, and N is the number of unit cells in the solid.

The solution of the Quantum Harmonic Oscilator (QHO) gives the relation between operators $a_{\mathbf{q},p}$ and the position operator, which is in this case given by

$$u^\nu_{\mathbf{q},\alpha,j} = \frac{1}{\sqrt{2M_\alpha\omega_{\mathbf{q},\nu}}}\varepsilon^\nu_{\alpha,j}(\mathbf{q})(a_{\mathbf{q},\nu} + a^\dagger_{-\mathbf{q},\nu}) \tag{7}$$

Here $\varepsilon^\nu_{\alpha,j}(\mathbf{q})$ (or $\vec{\varepsilon}^\nu_\alpha(\mathbf{q})$) is the phonon polarization, and M_α is the ionic mas at Wickoff position α.

When solving the phonon problem, we wrote the following equation

$$[H_e + \sum_{i,j} V_{e-i}(\mathbf{r}_j - \mathbf{R}_i) + \sum_{i\neq j} V_{i-i}(\mathbf{R}_i - \mathbf{R}_j)]\,|\psi_{electron}\rangle = E_{electron}[\{\mathbf{R}\}]\,|\psi_{electron}\rangle \tag{8}$$

which gives the solution of the electron problem in the static lattice approximation (Born-Oppenheimer), where $\mathbf{R}_i$ are lattice vectors of ions, H_e is the electron Hamiltonian, and V_{e-i} and V_{i-i} are electron-ion and ion-ion Coulomb repulsions, respectively.

Due to ionic vibrations, the displacement of ions creates an additional term in the Hamiltonian, which according to the above equation, should be proportional to

$$H_{e-i} = \int d^3r \sum_{n,\alpha} [V_{e-i}(\mathbf{r} - \mathbf{R}_{n\alpha} - \vec{u}_{n\alpha}) - V_{e-i}(\mathbf{r} - \mathbf{R}_{n\alpha})]\rho_{electron}(\mathbf{r}) \tag{9}$$

where $\mathbf{R}_{n\alpha}$ is position of an ion at Wickoff position α and unit cell n.

- Using above equations, shows that for small phonon-displacement u, the electron-phonon coupling should have the form

$$H_{e-i} = \sum_{\alpha,j,\mathbf{q},\nu,\sigma,i_1,i_2,\mathbf{k}} c^\dagger_{i_1,\mathbf{k}+\mathbf{q},\sigma}c_{i_2,\mathbf{k},\sigma}(a_{\mathbf{q},\nu} + a^\dagger_{-\mathbf{q},\nu})\frac{g^{\mathbf{k},\mathbf{q}}_{i_1,i_2,\alpha,\nu}}{\sqrt{2M_\alpha\omega_{\mathbf{q},\nu}}} \tag{10}$$

where the electron field operator is expanded in Bloch basis

$$\psi_\sigma(\mathbf{r}) = \sum_{\mathbf{k},i} \psi_{\mathbf{k},i}(\mathbf{r})c_{\mathbf{k},i,\sigma} \tag{11}$$

and the matrix elements g are given by

$$g^{\mathbf{k},\mathbf{q}}_{i_1,i_2,\alpha,\nu} = \frac{1}{\sqrt{N}}\sum_j \varepsilon^\nu_{\alpha,j}(\mathbf{q})\,\langle\psi_{\mathbf{k}+\mathbf{q},i_1}|\sum_n e^{i\mathbf{q}\mathbf{R}_n}\frac{\partial V_{e-i}(\mathbf{r} - \mathbf{R}_{n\alpha})}{\partial R_{n\alpha,j}}|\psi_{\mathbf{k},i_2}\rangle \tag{12}$$

Explain why the above integration $\langle\psi_{\mathbf{k}+\mathbf{q},i_1}|...|\psi_{\mathbf{k},i_2}\rangle$ can be carried over a single unit cell, or over the entire solid.

- Now use the following approximations to simplify the above Hamiltonian

* We have only one type of atom in the unit cell, i.e., $M_\alpha = M$.
* We consider only one Bloch band, i.e., $c_{i_1\mathbf{k}} = c_\mathbf{k}$ in our model.
* We consider the longitudinal phonon with $\omega_{\mathbf{q},\nu} = \omega_\mathbf{q}$ and approximate form

$$g_{i_1,i_2,\alpha,\nu}^{\mathbf{k},\mathbf{q}} \approx \delta_{i_1,i_2}\ iq_\nu\ \gamma. \tag{13}$$

Show that H_{e-i} is

$$H_{e-i} = \gamma \sum_{\nu,\mathbf{q},\sigma,\mathbf{k}} c_{\mathbf{k+q},\sigma}^\dagger c_{\mathbf{k},\sigma}(a_{\mathbf{q},\nu} + a_{-\mathbf{q},\nu}^\dagger)\frac{iq_\nu}{\sqrt{2M\omega_\mathbf{q}}} \tag{14}$$

- Introduce Grassmann field $\psi_{\mathbf{q}\sigma}$ for the coherent states of the electrons $c_{\mathbf{k}\sigma}$ and complex fields $\Phi_{\mathbf{q},j}$ for phonon operators $a_{\mathbf{q},j}$, and show that the action of the electron-phonon problem has the form

$$S = \int_0^\beta d\tau \sum_{\mathbf{k},\sigma} \psi_{\mathbf{k}\sigma}^\dagger(\partial_\tau + \varepsilon_\mathbf{k})\psi_{\mathbf{k}\sigma} + \int_0^\beta d\tau \sum_{\mathbf{q},\nu} \Phi_{\mathbf{q},\nu}^\dagger(\partial_\tau + \omega_\mathbf{q})\Phi_{\mathbf{q},\nu} \tag{15}$$

$$+\gamma \int_0^\beta \sum_{\nu,\mathbf{q},\sigma,\mathbf{k}} \psi_{\mathbf{k+q},\sigma}^\dagger \psi_{\mathbf{k},\sigma}(\Phi_{\mathbf{q},\nu} + \Phi_{-\mathbf{q},\nu}^\dagger)\frac{iq_\nu}{\sqrt{2M\omega_\mathbf{q}}} \tag{16}$$

- Introduce fields in Matsubara space ($\psi_{\mathbf{k}\sigma}(\tau) \to \psi_{\mathbf{k}\sigma,n}$ and $\Phi_{\mathbf{q},\nu}(\tau) \to \Phi_{\mathbf{q},\nu,m}$) to transform the action S to the diagonal form. Next, use the functional field integral technique to integrate out the phonon fields, and obtain the effective electron action of the form

$$S_{eff} = \sum_{\mathbf{k},\sigma,n} \psi_{\mathbf{k}\sigma,n}^\dagger(-i\omega_n + \varepsilon_\mathbf{k})\psi_{\mathbf{k}\sigma,n} - \frac{\gamma^2}{2M\beta} \sum_{\mathbf{q},n} \frac{q^2}{\omega_\mathbf{q}^2 + \Omega_n^2} n_{\mathbf{q},n} n_{-\mathbf{q},-n} \tag{17}$$

where the electron charge density is

$$n_{\mathbf{q},n} = \sum_{\mathbf{k},\sigma,m} \psi_{\mathbf{k+q},\sigma,m+n}^\dagger \psi_{\mathbf{k},\sigma,m} \tag{18}$$

Notice that at small frequency $\Omega_m \to 0$ this interaction is attractive, which is the necessary condition for the conventional superconductivity to occur.

Explain why ions with small mass (like hydrides with Hydrogen) could a"chieve high-Tc with conventional superconductivity. Somewhat counterintuitive is the requirement that the phonon frequency should be large (and not small), as naively suggested by the dimensional analysis. Comment why you think high phonon frequency might still be beneficial to superconductivity?

Finally a word of caution: In ab-initio calculations V_{e-i} should be the Kohn-Sham potential, rather than the bare Coulomb potential. This is because at low energy electrons feel the screened Coulomb repulsion as the electrons are very fast and adjust to the current position of phonons. The alternative formula, first derived by Bardeen, uses dynamically screened bare Coulomb repulsion $V_{e-i} = \varepsilon^{-1}(\omega)V_C$, instead of V_{KS}. The latter formula has received very little attention to date, because of difficulty of computing precise $\varepsilon_{\mathbf{r},\mathbf{r}'}^{-1}(\omega)$.

4) Show that the quantum impurity problem with the Hamiltonian

$$H = \sum_{s,\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k},s}^\dagger c_{\mathbf{k},s} + V_{\mathbf{k}} c_{\mathbf{k},s}^\dagger d_s + V_{\mathbf{k}}^* d_s^\dagger c_{\mathbf{k},s} + \varepsilon_d(n_{d\uparrow} + n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow} \qquad (19)$$

can be written in terms of action of the following form

$$S = \int_0^\beta d\tau \left[\sum_s \psi_s^\dagger(\tau)(\frac{\partial}{\partial \tau} + \varepsilon_d)\psi_s(\tau) + U n_{d\uparrow} n_{d\downarrow} \right] + \sum_s \int_0^\beta \int_0^\beta d\tau d\tau' \psi_s^\dagger(\tau)\Delta(\tau - \tau')\psi_s(\tau')(20)$$

Here $n_{ds} = \psi_s^\dagger \psi_s$, while above $n_{ds} = d_s^\dagger d_s$.

What is Δ?

Hint: integrate out the fermions $c_{\mathbf{k},s}$.

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