Karlsruher Institut für Technologie | Institut für Theorie der Kondensierten Materie

Microscopic Theory of Superconductivity WS 2014/15

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Sheet 02
Due date 24.11.2014

1. Electron-electron and electron-phonon interactions in jellium
$(20 + 20 = 40$ points)
The microscopic Hamiltonian of conduction electrons interacting electrostatically with core ions of charge $Z_c e_0$ in a solid is given by

$$H = H_e + H_i + H_{ei}$$
$$= \sum_i \frac{\boldsymbol{p}_i^2}{2m} + \frac{e_0^2}{2}\sum_{i\neq j}\frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \sum_\nu \frac{\boldsymbol{P}_\nu^2}{2M} + \frac{Z_i^2 e_0^2}{2}\sum_{\nu\neq\mu}\frac{1}{|\boldsymbol{R}_\nu - \boldsymbol{R}_\mu|} - Z_i e_0^2 \sum_{i,\nu}\frac{1}{|\boldsymbol{r}_i - \boldsymbol{R}_\nu|}\,.$$

The jellium model neglects the periodic lattice structure of the ions (plus core electrons) and considers the ionic system as a uniform background of positive charges with charge density $Z_i e_0 N_i/V$, where N_i is the number of core ions the system of volume V. The number of conduction electrons is equal to $N = Z_i N_i$ so that total system is charge neutral. The Hamiltonian of the jellium model is given by

$$H_{\text{jellium}} = \sum_i \frac{\boldsymbol{p}_i^2}{2m} + \frac{e_0^2}{2}\sum_{i\neq j}\frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \frac{Z_i^2 e_0^2 N^2}{2V^2}\int d^3R\, d^3R' \frac{e^{-\alpha|\boldsymbol{R}-\boldsymbol{R}'|}}{|\boldsymbol{R}-\boldsymbol{R}'|}$$
$$- \frac{Z_i e_0^2 N}{V}\sum_i \int d^3R \frac{e^{-\alpha|\boldsymbol{R}-\boldsymbol{R}'|}}{|\boldsymbol{r}_i - \boldsymbol{R}|} + H_{ph} + H_{e,ph}\,. \tag{1}$$

We have regularized the Coulomb potential by introducing an exponential factor, and have to take the limit $\alpha \to 0$ in the end. The parts $H_{ph} + H_{e,ph}$ describe the interaction of the oscillations of the ions, the phonons, with the electrons. We will deal with this part below.

(a) Write the Hamiltonian H_{jellium} in momentum space $\boldsymbol{q}$ with respect to the electron coordinate $\boldsymbol{r}_i$ and explicitly perform the integrations over $\boldsymbol{R}$ to show that the $\boldsymbol{q} = 0$ component of the electron-electron interaction vanishes (in the thermodynamic limit).

(b) One obtains the phonon H_{ph} and the electron-phonon part $H_{e,ph}$ of the Hamiltonian by expanding to lowest non-vanishing order in the deviations of the ions from the equilibrium positions $\delta\boldsymbol{R}_\nu = \boldsymbol{R}_\nu - \boldsymbol{R}_\nu^0 = \frac{1}{\sqrt{N_i M}}\sum_{\boldsymbol{q},\lambda} Q_{\boldsymbol{q}\lambda}\boldsymbol{\epsilon}_{\boldsymbol{q}\lambda}e^{i\boldsymbol{q}\boldsymbol{R}_\nu^0}$. Here, $\boldsymbol{\epsilon}_{\boldsymbol{q}\lambda}$ denotes the polarization vectors and $Q_{\boldsymbol{q}\lambda}$ the normal coordinates. Associated normal momentum coordinates are given by $\boldsymbol{P}_\nu = \left(\frac{M}{N_i}\right)^{1/2}\sum_{\boldsymbol{q},\lambda}\Pi_{\boldsymbol{q}\lambda}\boldsymbol{\epsilon}_{\boldsymbol{q}\lambda}e^{-i\boldsymbol{q}\boldsymbol{R}_\nu^0}$. They satisfy $[\Pi_{\boldsymbol{q}\lambda}, Q_{\boldsymbol{q}'\lambda'}] = -i\hbar\delta_{\boldsymbol{q}\boldsymbol{q}'}\delta_{\lambda\lambda'}$ and commute among themselves. We can introduce bosonic creation and annihilation operators as $Q_{\boldsymbol{q}\lambda} = \left(\frac{\hbar}{2\Omega_{\boldsymbol{q}\lambda}}\right)^{1/2}(a_{\boldsymbol{q}\lambda} + a^\dagger_{-\boldsymbol{q}\lambda})$ and $\Pi_{\boldsymbol{q}\lambda} = i\left(\frac{\hbar\Omega_{\boldsymbol{q}\lambda}}{2}\right)^{1/2}(a^\dagger_{\boldsymbol{q}\lambda} - a_{-\boldsymbol{q}\lambda})$. In terms of the normal coordinates the phonon and the electron-phonon part of the Hamiltonian take the form (in second quantization)

$$H_{ph} = \frac{1}{2}\sum_{\boldsymbol{q},\lambda}\Big(\Pi^\dagger_{\boldsymbol{q}\lambda}\Pi_{\boldsymbol{q}\lambda} + \Omega^2_{\boldsymbol{q}\lambda}Q^\dagger_{\boldsymbol{q}\lambda}Q_{\boldsymbol{q}\lambda}\Big) = \sum_{\boldsymbol{q},\lambda}\hbar\Omega_{\boldsymbol{q}\lambda}(a^\dagger_{\boldsymbol{q}\lambda}a_{\boldsymbol{q}\lambda} + \frac{1}{2}) \tag{2}$$

$$H_{e,ph} = \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma,\lambda} g_{\boldsymbol{k}\boldsymbol{k}'\lambda}(a_{\boldsymbol{k}'-\boldsymbol{k},\lambda} + a^\dagger_{\boldsymbol{k}-\boldsymbol{k}',\lambda})c^\dagger_{\boldsymbol{k}'\sigma}c_{\boldsymbol{k}\sigma}\,. \tag{3}$$

By expanding the electron-ion Coulomb interaction to linear order in $\delta\boldsymbol{R}_\nu$ obtain an explicit result for the electron-phonon matrix element $g_{\boldsymbol{k}\boldsymbol{k}'\lambda}$ within the jellium model. Note that the only the coupling to longitudinal phonons is non-zero.

2. Random phase approximation of Coulomb interaction in jellium
$(15+15+10+20=60$ points$)$
The free conduction electron system is described by the Hamilonian $H_{e,0} = \sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}$ with dispersion $\epsilon_{\boldsymbol{k}} = \boldsymbol{k}^2/2m$. The free phonon system is given in Eq. (2).

(a) Determine the time evoluation of the electron operators in the Heisenberg picture to calculate the free time-ordered Green function in real-time at zero temperature

$$G_0(\boldsymbol{k}\sigma,t) = -i\langle 0|T\big(c_{\boldsymbol{k}\sigma}(t)c^\dagger_{\boldsymbol{k}\sigma}(0)\big)|0\rangle\,. \tag{4}$$

Here, T denotes the time-ordering symbol and $|0\rangle$ denotes the many-body ground state at zero temperature with states below the Fermi wavevector $\boldsymbol{k}_F$ being filled and states above it being empty. Give the Green function in frequency space $G_0(\boldsymbol{k}\sigma,t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G_0(\boldsymbol{k}\sigma,\omega)e^{-i\omega t}$.

(b) Determine the time evoluation of the phonon operators in the Heisenberg picture to calculate the free time-ordered Green function in real-time at zero temperature

$$D_{0,\lambda}(\boldsymbol{q}\lambda,t) = -i\langle 0|T\big(\varphi_{\boldsymbol{q}\lambda}(t)\varphi^\dagger_{\boldsymbol{q}\lambda}(0)\big)|0\rangle\,, \tag{5}$$

where $\varphi_{\boldsymbol{q}\lambda}(t) = a_{\boldsymbol{q}\lambda}(t) + a^\dagger_{-\boldsymbol{q}\lambda}(t)$ and $|0\rangle$ denotes the zero temperature ground state of H_{ph}.

(c) Write down the bare Coulomb interaction Hamiltonian in momentum space in second quantized form (using your results from exercise 1).

(d) The main screening effects of the Coulomb interaction arise from the bubble diagrams shown in the figure. Summing over all the bubble diagrams amounts to the so-called RPA approximation

$$V_{RPA}(\boldsymbol{q},\omega) = V(\boldsymbol{q}) - V(\boldsymbol{q})P_{RPA}(\boldsymbol{q},\omega)V_{RPA}(\boldsymbol{q},\omega) \tag{6}$$

with $P_{RPA}(\boldsymbol{q},\omega_0) = 2i\int\frac{d\omega d^3p}{(2\pi)^4}G_0(\boldsymbol{p}+\boldsymbol{q},\omega+\omega_0)G_0(\boldsymbol{p},\omega)$. Write the screened interaction as $V_{RPA}(\boldsymbol{q},\omega) = V(\boldsymbol{q})/\epsilon(\boldsymbol{q},\omega)$ and determine $\epsilon(\boldsymbol{q},\omega)$. Determine in which region Imϵ becomes non-zero. Disuss the cases $\epsilon(\boldsymbol{q},0)$, $\epsilon(|\boldsymbol{q}_F|,0$ and $\epsilon(|\boldsymbol{q}\to\infty,\omega)$.