[8] Electron-Phonon Interaction and BCS Hamiltonian

∘ We assume that the positive and the negative charges are almost equally distributed:

$$n_+(x) = \bar{n} + \Delta n_+ \qquad n_-(x) = \bar{n} + \Delta n_- \quad \text{—①}$$

∘ We assume that the excess energy caused by the density fluctuation is proportional to

$$\Delta \epsilon(x) \approx -\kappa \, \Delta n_+ \Delta n_- \qquad (\text{per volume}) \quad \text{—②}$$

in the neighborhood of x, which is reasonable from the original Coulomb's law.

∘ Of cause, the assumption of the almost uniform distribution ① is obviously wrong. However, it would be not so unrealistic to assume the form ② considering Δn_+, Δn_- as the deviation from the stable charge neutral distribution. Another implicit assumption : "The effect of the positive charge distribution on the electrons can be described by the continuous distribution function $\Delta n_+(x)$". can be also justified (retrospectively) by the fact that the Cooper pair is typically much larger than the lattice constant ; the electrons feel the averaged influence from the positive ions.

even if it's not uniform

- By introducing the displacement vector of an positive ion $\mathbf{u}(\mathbf{x})$ the local density fluctuation of the positive ions can be written as

$$\Delta n_+ = -\bar{n}\,(\nabla\cdot\mathbf{u}(\mathbf{x}))$$ ($\mathbf{u}$ was previously denoted as $\mathbf{q}$)

- By the electron field operators, $\hat{\psi}(\mathbf{x})$, the local density fluctuation of the electrons is

$$\Delta n_- = \sum_{\sigma=\uparrow,\downarrow} \hat{\psi}^\dagger_\sigma(\mathbf{x})\,\hat{\psi}_\sigma(\mathbf{x}) - \bar{n}$$

- The excess energy is $\varkappa\,\bar{n}\,(\nabla\cdot\mathbf{u})\left(\sum_\sigma\hat{\psi}^\dagger\hat{\psi} - \bar{n}\right)$, so,

$$\Delta E = \varkappa\,\bar{n}\,(\nabla\cdot\mathbf{u})\sum_\sigma \hat{\psi}^\dagger_\sigma\hat{\psi}_\sigma$$

since the term $\varkappa\,\bar{n}^2\,\nabla\cdot\mathbf{u}$, when integrated, is reduced to a surface integral and can be dropped.

- By Fourier expanding $\mathbf{u}(\mathbf{x})$, we get,

$$\mathbf{u}(\mathbf{x}) = \frac{1}{\sqrt{\Lambda}}\sum_{\mathbf{q}} \mathbf{u}\; e^{i\mathbf{q}\cdot\mathbf{x}} \qquad \left(\Lambda \equiv \frac{L^d}{a^d}\right)$$

Here we can assume the longitudinal wave, i.e., $\mathbf{u}_{\mathbf{k}} \parallel \mathbf{k}$ since the transverse mode does not contribute to $\nabla\cdot\mathbf{u}$. So we have

$$\mathbf{u}(\mathbf{x}) = \frac{1}{\sqrt{\Lambda}}\sum_{\mathbf{q}} \hat{\mathbf{q}}\,u_{\mathbf{q}}\,e^{i\mathbf{q}\cdot\mathbf{x}} \qquad \left(\hat{\mathbf{q}} \equiv \frac{\mathbf{q}}{|\mathbf{q}|}\right)$$

As we did before by introducing the phonon creation/annihilation operators by

$$u_q = \sqrt{\frac{\hbar}{2m\omega_q}}\,(b_q^+ + b_q)$$

$$P_q = i\sqrt{\frac{m\hbar\omega_q}{2}}\,(b_q^+ - b_q)$$

the phonon Hamiltonian is $\sum_q \hbar\omega_q (b_q^+ b_q + \frac{1}{2})$

The the electron-phonon interaction term in question will be

$$\mathcal{H}_{el-ph} = \sum_x \Delta\epsilon(x)$$

$$= \sum_{x,\sigma} \kappa\bar{n}\,(\nabla\cdot u)\,\hat{\psi}_\sigma^+ \hat{\psi}_\sigma$$

$$= \kappa\bar{n} \sum_{x,\sigma}\left(\frac{1}{\sqrt{\Omega}}\sum_q \hat{q}\sqrt{\frac{\hbar}{2m\omega_q}}\,(\nabla e^{iq\cdot x})(b_q^+ - b_q)\right)$$

$$\times \frac{1}{\Omega}\sum_{k k'} e^{-i(k'-k)\cdot x}\, c_{k'\sigma}^+ c_{k\sigma}$$

$$\left(\hat{\psi}_\sigma(x) \equiv \frac{1}{\sqrt{\Omega}}\sum_k e^{ik\cdot x} c_{k\sigma}\right)$$

$$= i\,\kappa\bar{n}\frac{1}{\sqrt{\Omega}}\sum_\sigma\sum_{k\,q}\sqrt{\frac{\hbar}{2m\omega_q}}\,q\,(b_q^+ - b_q)\,c_{k+q\,\sigma}^+ c_{k\sigma}$$

$$= \frac{1}{\sqrt{\Omega}}\sum_{k q \sigma} i\,\alpha_q\, c_{k+q,\sigma}^+ c_{k,\sigma}\,(b_q^+ - b_q)$$

$$\alpha_q \equiv \kappa\bar{n}\sqrt{\frac{\hbar}{2m\omega_q}}\,|q| \quad \left(\propto \sqrt{q} \quad (\because \omega_q \propto |q|)\right)$$

BCS Hamiltonian

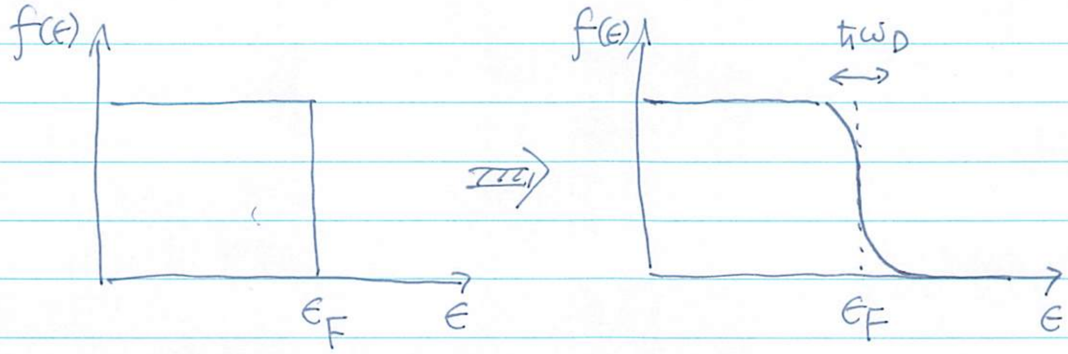
We consider the situation where the electrons and the phonons are weakly-coupled at zero temperature. We will derive an effective interaction among the electrons by the 2nd order perturbative approximation with respect to the electron-phonon coupling.

However, as we see below, our argument, following the BCS theory, will eventually lead to a result that is dramatically different from the non-perturbative system, beyond any perturbative approximation. Therefore, the perturbative treatment in deriving the effective interaction may seem self-contradicting.

This apparent logical flaw may be removed by viewing the effective attraction among electrons as valid not only for the non-pertubative system but also for the set of states, i.e., ansatz, that the final state may belong to.

More specifically, we assume that the true ground state in the presence of the electron-phonon interaction is the state that is not far from the non-perturbative state (i.e. fermi sea + phonon vacuum) in that electrons still have the fermi-sea-like distribution with a "blurred" fermi-surface to the width of $\hbar\omega_D$ (Debye frequency) and phonons exist only as virtual ones mediating electron-electron attraction.

non-perturbative BCS



These properties are trivially applicable to non-perturbative state. The property that the fermi surface is blurred by $\hbar\omega_D$ may be reasonable since an electron colliding with a phonon change its energy by $\hbar\omega_D$ typically.
However, many things are not clear a priori, e.g., we cannot tell whether other effective interaction that would arize from even higher perturbations change the whole story or not.

We can only say that the present treatment is at least not self-contradicting. As long as it is not self-inconsistent, there is a chance for it to be right. Whether it is really right or not must be checked by comparison with experiment or more sofisticated theories.

○ The second order perturbation

Our Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + V$
where $\mathcal{H}_0$ is the non-interaction electron system for which the Fermi sea is the ground state, and V is the electron-phonon coupling.

We want to derive effective interaction among electrons mediated by the phonons. To this end, we'll apply a unitary transformation to the whole system so that the electrons and the phonons are decoupled (up to the second order in V.).

$$U = e^{iP} \quad (P^+ = P)$$

$$\tilde{\mathcal{H}} \equiv U^+ \mathcal{H} U = e^{-iP} \mathcal{H} e^{iP} \qquad (P = \mathcal{O}(V))$$

$$= e^{-iP^\times} \mathcal{H}$$

($P^\times$ is a super operator such that $P^\times A = [P, A]$ for any operator A)

$$= \mathcal{H} - i[P, \mathcal{H}] - \frac{1}{2}[P, [P, \mathcal{H}]] + \mathcal{O}(V^3)$$

$$= \mathcal{H}_0 + (V - i[P, \mathcal{H}_0])$$

$$- i[P, V] - \frac{1}{2}[P, [P, \mathcal{H}_0]] + \mathcal{O}(V^3)$$

Therefore, if we choose P so that

$$[P, \mathcal{H}_0] = \frac{1}{i} V \qquad \text{①}$$

$$\tilde{\mathcal{H}} = \mathcal{H}_0 - i[P, V] - \frac{1}{2}[P, \frac{1}{i}V] + O(V^3)$$

$$= \mathcal{H}_0 - \frac{i}{2}[P, V] + O(V^3) \quad \text{—— ②}$$

In the basis system that diagonalize $\mathcal{H}_0$ (i.e. $\langle m|\mathcal{H}_0|n\rangle = \delta_{mn}E_m$), Eq. ① is

$$P_{mn}E_n - E_m P_{mn} = -iV_{mn}$$

$$\longrightarrow \quad P_{mn} = \frac{iV_{mn}}{E_m - E_n}$$

Then Eq. ② tells us that

$$\tilde{\mathcal{H}}_{mn} = (\mathcal{H}_0)_{mn} - \frac{i}{2}\sum_l (P_{ml}V_{ln} - V_{ml}P_{ln})$$

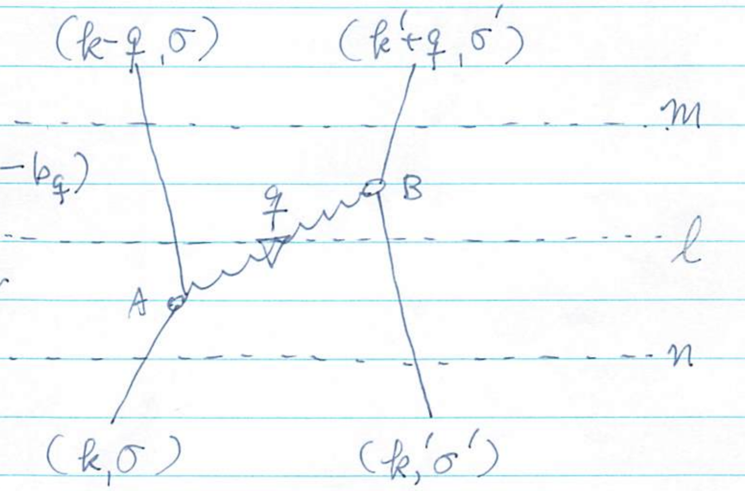
$$= (\mathcal{H}_0)_{mn} + \frac{1}{2}\sum_l \left(\frac{1}{E_m - E_l} - \frac{1}{E_l - E_n}\right)V_{ml}V_{ln}$$

$$\tilde{\mathcal{H}}_{mn} = (\mathcal{H}_0)_{mn} - \frac{1}{2}\sum_l \left(\frac{1}{E_l - E_m} + \frac{1}{E_l - E_n}\right)V_{ml}V_{ln}$$

Here, we recall that

$$V = \frac{1}{\sqrt{\Omega}}\sum_{kq\sigma} i\alpha_q c^\dagger_{k+q\sigma}c_{k\sigma}(b^\dagger_{-q} - b_q)$$

and in the state we consider the phonons can exist only as the virtual ones, and the Fermi sea is modified only in the vicinity of the Fermi surface.



It follows that the electron-phonon interaction affects the electron only as dipicted in the diagram. with q in the range $-q_D < |q| < q_D$ (q_D: "Debye" wave number ($q_D = \omega_D/c \doteq \pi/a$))

The vertex A corresponds to $\Lambda^{-\frac{1}{2}} i\alpha_{-q} c^{+}_{k-q} c_k b^{+}_q$, and the vertex B corresponds to $-\Lambda^{-1/2} i\alpha_q c^{+}_{k'+q} c_{k'} b_q$

$$E_m = \overbrace{\epsilon_{k-q}}^{(\mathrm{const}+} + \epsilon_{k'+q} \qquad E_n = \epsilon_k + \epsilon_{k'}$$

$$E_l = \epsilon_{k-q} + \epsilon_{k'} + \hbar\omega_q$$

Therefore,

$$\tilde{\mathcal{H}} = \mathcal{H}_0 - \frac{1}{2}\sum_{\substack{q\,kk'\\ \sigma\sigma'}} \left(\frac{1}{\epsilon_{k'} + \hbar\omega_q - \epsilon_{k'+q}} + \frac{1}{\epsilon_{k-q} + \hbar\omega_q - \epsilon_k} \right) \times \frac{|\alpha_q|^2}{\Lambda} c^{+}_{k'+q} c_{k'} c^{+}_{k-q} c_k \underbrace{b_q b^{+}_q}_{=1\ (\because \text{Ansatz})}$$

$$= (\mathcal{H}_0)_{mn} - \frac{1}{4}\sum_{\substack{kk'q\\ \sigma\sigma'}} \frac{|\alpha_q|^2}{\Lambda} \left[\left(\frac{1}{\epsilon_{k'} + \hbar\omega_q - \epsilon_{k'+q}} + \frac{1}{\epsilon_{k-q} + \hbar\omega_q - \epsilon_k} \right) \times c^{+}_{k'+q\,\sigma'} c_{k'\sigma'} c^{+}_{k-q\,\sigma} c_{k\sigma} + (k \leftrightarrow k' \ \ q \leftrightarrow -q) \right]$$

$$= (\mathcal{H}_0)_{mn} - \frac{1}{4}\sum_{\substack{kk'q\\ \sigma\sigma'}} \frac{|\alpha_q|^2}{\Lambda} c^{+}_{k'+q\,\sigma'} c_{k'\sigma'} c^{+}_{k-q\,\sigma} c_{k\sigma} \times \left[\frac{1}{\epsilon_{k'} + \omega_q - \epsilon_{k'+q}} + \frac{1}{\epsilon_{k-q} + \omega_q - \epsilon_k} + \frac{1}{\epsilon_k + \omega_q - \epsilon_{k-q}} + \frac{1}{\epsilon_{k'+q} + \omega_q - \epsilon_{k'}} \right]$$