Lecture VIII: Electron-phonon interaction and Cooper instability

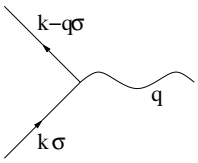
▷ History:

- 1911 discovery of superconductivity
- 1951 "isotope effect" — clue to (conventional) mechanism
- 1957 BCS theory of conventional superconductivity
- 1986 Discovery of unconventional superconductivity in cuprates
- ???? awaiting theory?

▷ (Conventional) mechanism: exchange of phonons can induce (non-local) attractive pairwise interaction between electrons

Electron pairs can condense into macroscopic phase coherent state with energy gap to quasi-particle excitations

▷ How does phonon exchange mediate interaction...?



Electron-phonon interaction:

$$\hat{H} = \overbrace{\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a^\dagger_{\mathbf{q}} a_{\mathbf{q}}}^{\hat{H}_0} + \overbrace{\sum_{\mathbf{k},\mathbf{q}} \left(M_{\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma} a_{\mathbf{q}} + \text{h.c.} \right)}^{\hat{H}_1}$$

simplicity: assume $M_{\mathbf{q}} = M$ constant

Effective Hamiltonian: eliminate phonons by canonical transformation
$\hat{H} \longmapsto \hat{H}' = e^{-\hat{S}} \hat{H} e^{\hat{S}}$ (cf. second order perturbation theory)

$$e^{-\hat{S}} \hat{H} e^{\hat{S}} = \hat{H} + [\hat{H}, \hat{S}] + \frac{1}{2}[[\hat{H}, \hat{S}], \hat{S}] + \cdots$$

"Schrieffer-Woolf transformation"

Terms 1st order in M eliminated by setting $\hat{H}_1 + [\hat{H}_0, \hat{S}] = 0$, viz.

$$\hat{H}' = \hat{H}_0 + \frac{1}{2}\left[\hat{H}_1, \hat{S}\right] + O(M^3)$$

In basis of non-interacting Hamiltonian: $|n\rangle = |\{\mathbf{k}\}\rangle_{\text{el.}} \otimes |\{\mathbf{q}\}\rangle_{\text{ph.}}$, $\{E_n\} = \{\epsilon_k + \hbar\omega_q\}$

$$\langle n|\hat{H}_1|m\rangle = \langle n|\hat{S}\hat{H}_0 - \hat{H}_0\hat{S}|m\rangle = (E_m - E_n)\langle n|\hat{S}|m\rangle$$
$$\langle n|\hat{S}|m\rangle = \frac{\langle n|\hat{H}_1|m\rangle}{E_m - E_n},$$

i.e. $$\langle n|\hat{H}'|m\rangle = \langle n|\hat{H}_0|m\rangle + \sum_p \langle n|\hat{H}_1|p\rangle\langle p|\hat{H}_1|m\rangle \left[\frac{1}{E_m - E_p} + \frac{1}{E_n - E_p}\right] + O(M^3)$$

In operator form,

$$\begin{aligned}\hat{H}' &= \hat{H}_0 + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{|M|^2}{2}\left\{\frac{1}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}}) - \hbar\omega_{\mathbf{q}}} + \frac{1}{(\epsilon_{\mathbf{k}'+\mathbf{q}} - \epsilon_{\mathbf{k}'}) - \hbar\omega_{\mathbf{q}}}\right\} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}-\mathbf{q}\sigma} c_{\mathbf{k}\sigma} \\ &= \hat{H}_0 + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} |M|^2 \frac{\hbar\omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2 - \hbar^2\omega_{\mathbf{q}}^2} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}-\mathbf{q}\sigma} c_{\mathbf{k}\sigma}.\end{aligned}$$

translates to an attractive (i.e. negative) interaction for excitation energies
in range $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}}| < \hbar\omega_{\mathbf{q}}$, and repulsive otherwise

N.B. consistency: truncate $\omega_{\mathbf{q}}$ sum at Debye frequency, $\omega_D \simeq q_{\max} v_S$
maximum quantum that can be excited among lattice modes

▷ Cooper instability

Consider two electrons propagating above a filled Fermi sea:

Is a weak pairwise interaction $V(\mathbf{r}_1 - \mathbf{r}_2)$ sufficient to create a bound state of pair?

Consider variational state

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \overbrace{\frac{1}{\sqrt{2}}(|\uparrow_1\rangle \otimes |\downarrow_2\rangle - |\uparrow_2\rangle \otimes |\downarrow_1\rangle)}^{\text{spin singlet}} \overbrace{\sum_{|\mathbf{k}|\geq k_F} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}}^{\text{spatial symm. } g_{\mathbf{k}} = g_{-\mathbf{k}}}$$

Applied to Schrödinger equation: $\hat{H}\psi = E\psi$

$$\sum_{\mathbf{k}} g_{\mathbf{k}} \left[2\epsilon_{\mathbf{k}} + V(\mathbf{r}_1 - \mathbf{r}_2)\right] e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)} = E \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}$$

Fourier transforming equation: $\times L^{-d} \int d(\mathbf{r}_1 - \mathbf{r}_2) e^{-i\mathbf{k}'\cdot(\mathbf{r}_1 - \mathbf{r}_2)}$

$$\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} g_{\mathbf{k}'} = (E - 2\epsilon_{\mathbf{k}}) g_{\mathbf{k}}, \qquad V_{\mathbf{k}\mathbf{k}'} = \int d\mathbf{r}\, V(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

If we assume

$$V_{\mathbf{k}\mathbf{k}'} = \begin{cases} -V & \{|\epsilon_{\mathbf{k}} - \epsilon_F|, |\epsilon_{\mathbf{k}'} - \epsilon_F|\} < \omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} -V \sum_{\mathbf{k}'} g_{\mathbf{k}'} &= (E - \epsilon_{\mathbf{k}}) g_{\mathbf{k}} \\ -V \sum_{\mathbf{k}} \frac{1}{E - 2\epsilon_{\mathbf{k}}} \sum_{\mathbf{k}'} g_{\mathbf{k}'} &= \sum_{\mathbf{k}} g_{\mathbf{k}} \\ -V \sum_{\mathbf{k}} \frac{1}{E - 2\epsilon_{\mathbf{k}}} &= 1 \end{aligned}$$

$$V\sum_{\mathbf{k}}\frac{1}{2\epsilon_{\mathbf{k}}-E}\simeq\nu(\epsilon_F)V\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{d\epsilon}{2\epsilon-E}=\frac{\nu(\epsilon_F)V}{2}\ln\left(\frac{2\epsilon_F+2\hbar\omega_D-E}{2\epsilon_F-E}\right)=1$$

In limit of weak coupling, i.e. $\nu(\epsilon_F)\lambda\ll 1$

$$E\simeq 2\epsilon_F-2\hbar\omega_D e^{-\frac{2}{\lambda\nu(\epsilon_F)}}$$

- i.e. pair forms a bound state (no matter how small interaction!)
- energy of bound state is non-perturbative in $\nu(\epsilon_F)\lambda$

Radius of pair wavefunction: $g(\mathbf{r})=\sum_{\mathbf{k}}g(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}$

$$\langle r^2\rangle=\frac{\int d\mathbf{r}\mathbf{r}^2|g(\mathbf{r})|^2}{\int d\mathbf{r}|g(\mathbf{r})|^2}=\frac{\sum_{\mathbf{k}}|\nabla_{\mathbf{k}}g(\mathbf{k})|^2}{\sum_{\mathbf{k}}|g(\mathbf{k})|^2}\simeq\frac{v_F^2\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{4d\epsilon}{(2\epsilon-E)^4}}{\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{d\epsilon}{(2\epsilon-E)^2}}=\frac{4}{3}\frac{v_F^2}{(2\epsilon_F-E)^2}$$

if $2\epsilon_F-E\sim k_{\rm B}T_c$, $T_c\sim 10{\rm K}$, $v_F\sim 10^8{\rm cm/s}$, $\xi_0=\langle r^2\rangle^{1/2}\sim 10^4\mathring{A}$,
i.e. other electrons must be important

▷ BCS wavefunction

two electrons in a paired state has wavefunction

$$\phi(\mathbf{r}_1-\mathbf{r}_2)=(|\uparrow_1\rangle\otimes|\downarrow_2\rangle-|\downarrow_1\rangle\otimes|\uparrow_2\rangle)g(\mathbf{r}_1-\mathbf{r}_2)$$

with zero centre of mass momentum

Drawing analogy with Bose condensate, let us examine variational state

$$\psi(\mathbf{r}_1\cdots\mathbf{r}_{2N})=\mathcal{N}\prod_{n=1}^{N}\phi(\mathbf{r}_{2n}-\mathbf{r}_{2n-1})$$

Is state compatible with Pauli principle? Using $g(\mathbf{r}_1-\mathbf{r}_2)=\sum_{\mathbf{k}}g_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$
or, in second quantised form,

$$\int\frac{d\mathbf{r}_1}{L^d}\int\frac{d\mathbf{r}_2}{L^d}g(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}a_\uparrow^\dagger(\mathbf{r}_1)a_\downarrow^\dagger(\mathbf{r}_2)|\Omega\rangle=\sum_{\mathbf{k}}g_{\mathbf{k}}c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger|\Omega\rangle$$

then, of the terms in the expansion of

$$|\psi\rangle=\prod_{n=1}^{N}\left[\sum_{\mathbf{k}_n}g_{\mathbf{k}_n}c_{\mathbf{k}_n\uparrow}^\dagger c_{-\mathbf{k}_n\downarrow}^\dagger\right]|\Omega\rangle$$

those with all $\mathbf{k}_n$s different survive

Generally, more convenient to work in grand canonical ensemble
where one allows for (small) fluctuations in the total particle density

$$|\psi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle$$

i.e. statistical independence of pair occupation

Normalisation demands $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$ (exercise) while constraint in particle number leads to $\sum_{\mathbf{k}} v^2_{\mathbf{k}} = 2N$

In non-interacting electron gas $v_{\mathbf{k}} = \begin{cases} 1 & |\mathbf{k}| < k_F \\ 0 & |\mathbf{k}| > k_F \end{cases}$

expect interactions to smear Fermi surface
to balance kinetic and potential energies from pairing

Furthermore,

$$\langle\psi|(\hat{N} - N)^2|\psi\rangle = 2\left(\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}\right)^{1/2} \sim N^{1/2}\left(\frac{\omega_D}{\epsilon_F}\right)^{1/2} \ll N$$

To determine the variational parameters $v_{\mathbf{k}}$, one can use a variational principle, i.e. to minimise

$$\langle\psi|\hat{H} - \epsilon_F \hat{N}|\psi\rangle$$

▷ BCS Hamiltonian: However, since we are interested in both the ground state energy, and the spectrum of quasi-particle excitations, we will follow a different route and explore a simplified model Hamiltonian

$$\hat{H}_{\rm BCS} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$

in a mean-field approximation — formally equivalent to variational analysis (where appropriate)