

Superconductivity Part 3 Version 1

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Overview

We will examine the 2-electron theory of the origin of Cooper pairs and will obtain the effective Hamiltonian (Annett).

The 2-electron theory

Bloch energies

Phonons

Perturbation theory

Section 1

Bloch energies

Bloch – The periodic potential

- ▶ This section follows the notes in <https://billcelmaster.com/wp-content/uploads/2025/05/Conductivity-Part-3-V2.pdf>
- ▶ The Hamiltonian for an electron in a periodic array (in equilibrium):

$$H_P \psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi$$

where $V(\mathbf{r} + \mathbf{a}) = V(\mathbf{r})$.

- ▶ Bloch's theorem: All eigensolutions are of the form

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

where $u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$.

- ▶ There are N allowed wavelengths per primitive reciprocal cell.

Section 2

Phonons

Phonons – Lancaster 2.4

- ▶ Start with a lattice (crystal) of N atoms interacting as LHO's.

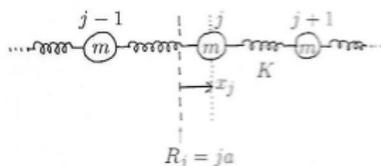


Fig. 2.5 A linear chain of atoms.

- ▶ The Hamiltonian is

$$\hat{H} = \sum_j \frac{\hat{p}_j^2}{2M} + \frac{1}{2}K (\hat{x}_{j+1} - \hat{x}_j)^2$$

where \hat{x}_j and \hat{p}_j are operators such that $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$.

- ▶ We can rewrite this by Fourier transforming the lattice, so writing

$$\hat{x}_j = \frac{1}{2\sqrt{N}} \sum_k \left[\tilde{\hat{x}}_k e^{ikja} + \text{hermitian conjugate} \right]$$
$$\hat{p}_j = \frac{1}{2\sqrt{N}} \sum_k \left[\tilde{\hat{p}}_k e^{ikja} + \text{hermitian conjugate} \right]$$

where $a = \frac{2\pi}{N}$.

Phonons – Lancaster 2.4 cont'd

- ▶ Lancaster then derives

$$\hat{H} = \sum_k \left[\frac{1}{2M} \tilde{p}_k \tilde{p}_{-k} + \frac{1}{2} M \omega_k^2 \tilde{x}_k \tilde{x}_{-k} \right]$$

where $\omega_k^2 = \left(\frac{4K}{M}\right) \sin^2\left(\frac{ka}{2}\right)$

- ▶ This form looks more factored (no differences of position or momentum)
- ▶ Define ladder operators $\hat{a}_j, \hat{a}_k^\dagger$ by

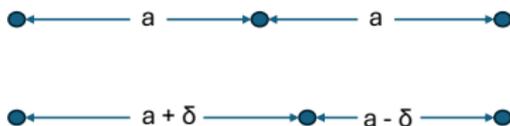
$$\hat{a}_k = \sqrt{\frac{M\omega_k}{2}} \left(\tilde{x}_k + \frac{i}{M\omega_k} \tilde{p}_k \right)$$

- ▶ Note that $[\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}$.
 - ▶ For Fermions, anticommutators would replace commutators.
- ▶ Then finally (see Lancaster)

$$\hat{H} = \sum_k \omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right)$$

Phonons – Coulomb potential between ions

- ▶ The real problem isn't a set of LHO's.
- ▶ Instead, ions with Coulomb forces shifted from equilibrium



- ▶ In equilibrium $V = \frac{e^2}{2\pi\epsilon_0 a}$.
- ▶ With δ displacement, $V = \frac{ke^2}{a+\delta} + \frac{ke^2}{a-\delta}$.
- ▶ Taylor expand: $V = \frac{e^2}{2\pi\epsilon_0 a} \left(1 + \frac{\delta^2}{a^2} + \dots \right)$
- ▶ We see that change from equilibrium is $\Delta V \approx \frac{e^2}{2\pi\epsilon_0 a^3} \delta^2$.
- ▶ Looks like LHO so we can apply the LHO analysis.

Phonons – Displacement operators

- ▶ This follows Annett Chapter 6
- ▶ Start with the original LHO model
 - ▶ From the definition of ladder operators $\tilde{\hat{x}}_k = \sqrt{\frac{\hbar}{2M\omega_k}} (\hat{a}_k + \hat{a}_k^\dagger)$
 - ▶ Fourier transform (including Hermitian conjugation)¹

$$\hat{x}_j = \sum_q \sqrt{\frac{\hbar}{2M\omega_q}} [a_q^\dagger + a_{-q}] e^{iqja}$$

- ▶ Now model a lattice with Coulomb-induced displacements.

$$\delta R_j = \sum_q \sqrt{\frac{\hbar}{2M\omega_q}} [a_q^\dagger + a_{-q}] e^{iqja}$$

¹l may be off by a factor of 2 and maybe a factor of \sqrt{N}

Phonons - Effect on electrons

- ▶ Lattice vibrations deform the periodic potential by δV .
 - ▶ Called the “deformation potential” $\delta V = \frac{\partial V}{\partial R_i} \delta R_i$
- ▶ The deformed potential modifies force on electron and its motion.
- ▶ In turn, the changed electron further deforms the inter-ion potential.
- ▶ That extra deformation causes extra modification on other electrons.
- ▶ According to Feynman, Statistical Physics, the induced $e^- - e^-$ interaction is “a consequence of one electron distorting the lattice, which in turn affects another electron”
- ▶ So δV essentially “acts twice” to cause an $e^- - e^-$ interaction.

Section 3

Perturbation theory

Perturbations: General QM

- ▶ How do we compute the “double action” of δV ?
- ▶ Let $H^{\text{tot}} = H_0 + V + \delta V$ where V is the periodic potential.
- ▶ $H_0 + V$ has eigenvalues E_k^0 with eigenstates $|k^{(0)}\rangle$.
- ▶ The second-order correction (Lippman Schwinger) to $H_0 + V$ is

$$\langle m^{(0)} | \delta H^{(2)} | n^{(0)} \rangle = \sum_{k \neq m} \frac{\langle m^{(0)} | \delta V | k^{(0)} \rangle \langle k^{(0)} | \delta V | n^{(0)} \rangle}{E_m^{(0)} - E_k^{(0)}}$$

where $E_m^{(0)} = E_n^{(0)}$.

Perturbations: Feynman Diagrams

- ▶ From Feynman Statistical Physics p. 271

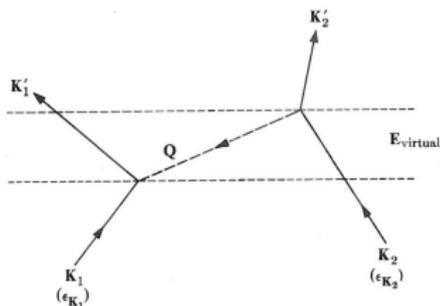


Fig. 10.7 One electron distorts the lattice, the other is affected by the distortion.

$$K'_1 - K_1 = Q,$$

$$K_2 - K'_2 = Q.$$

The initial energy is $E_{\text{initial}} = \varepsilon_{K_1} + \varepsilon_{K_2}$ in the intermediate region, and the virtual energy is

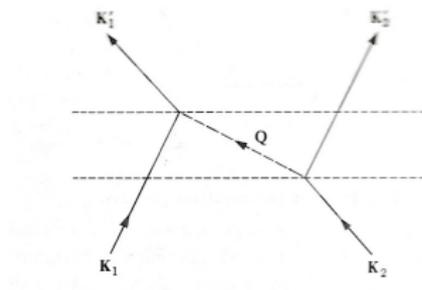
$$E_{\text{virtual}} = \varepsilon_{K'_1} + \varepsilon_{K'_2} + \hbar\omega_Q.$$

The perturbation energy due to the mechanism of Fig. 10.7 is

$$\begin{aligned} V_1 &= M_{K_2 K'_2} \frac{1}{E_{\text{initial}} - E_{\text{virtual}}} M_{K'_1 K_1}^* \\ &= M_{K_2 K'_2} \frac{1}{(\varepsilon_{K_1} + \varepsilon_{K_2}) - (\varepsilon_{K'_1} + \varepsilon_{K'_2} + \hbar\omega_Q)} M_{K'_1 K_1}^*. \end{aligned} \quad (10.6)$$

Perturbations: Feynman Diagrams cont'd

- ▶ Also add contribution from



- ▶ Take all energies ϵ_k near ϵ_F so we are left with

$$\langle k_1 k_2 | \delta H^{(2)} | k_1' k_2' \rangle \approx -\frac{1}{\hbar\omega_q} \left(M_{k_2 k_2'} M_{k_1' k_1}^* + M_{k_1 k_1'} M_{k_2' k_2}^* \right)$$

- ▶ Assume M 's are approximately equal
 - ▶ \implies perturbation energy is negative (attractive)
- ▶ Migdal estimated that the interaction vertex coupling $\propto \sqrt{\frac{m_e}{M}}$.
 - ▶ Makes sense because electron shouldn't move ion much

Perturbations: The screened Coulomb potential

- ▶ The Coulomb $e^- - e^-$ potential is $V_C(r) = \frac{e^2}{4\pi\epsilon_0 r}$.
- ▶ In Fourier space this becomes $\tilde{V}_C(q) = \frac{e^2}{\epsilon_0 q^2}$.
- ▶ Consider interaction of a conduction electron with e^- in Fermi sea
 - ▶ How does it effect an electron with energy $\epsilon_F - \delta$?
 - ▶ Suppose electrons are far apart so potential is $< \delta$.
 - ▶ Second electron can't change state because all nearby states are occupied.
 - ▶ So long-range Coulomb force is screened.
 - ▶ Modeled as a Yukawa-style potential $V_Y(r) = \frac{e^2 e^{-\alpha r}}{4\pi\epsilon_0 r}$
- ▶ So in Fourier space the screened potential is $\tilde{V}_Y(q) = \frac{e^2}{\epsilon_0(q^2 + \alpha^2)}$

Perturbations: Putting it all together

- ▶ The treatment of perturbation theory was a bit loopy-goopy.
 - ▶ However, it follows Feynman's way of thinking.
 - ▶ In a systematic approach, the interaction is of the form

$$\delta V = \sum_{k_1 k_2 k'_1 k'_2 q} c_{k_1}^\dagger c_{k_2}^\dagger a_q^\dagger a_{-q} c_{k'_1} c_{k'_2}$$

subject to certain constraints on the momenta.

- ▶ Interpret as a sum of operators where two electrons (“c” operators) transition from momenta k_1, k_2 , by exchanging a phonon (“a” operators) with momentum q , to momenta k'_1, k'_2 .
 - ▶ Above, all the operators act on a free-particle Hilbert space.
 - ▶ The original Hamiltonian involves interacting operators.
 - ▶ For “effective Hamiltonian” for electrons, integrate out phonons
- ▶ Coulomb is repulsive. A Cooper pair requires attractive potential.
 - ▶ At long range i.e. small frequency ($\omega < \omega_D$), phonon exchange is more attractive.
 - ▶ The effective H interaction term adds Coulomb plus phonon piece

$$H_I = -\kappa^2 \sum_{qkk'} c_{(k+q)\uparrow}^\dagger c_{(-k+q)\downarrow}^\dagger c_{(k'+q)\uparrow} c_{(-k'+q)\downarrow}$$