

→ Superconductivity:

⇒ Macroscopic prop.: → $\sigma = \infty$ / $\rho = 0$ $T < T_c$

→ $\chi = -1$ ← defining charact. SC

→ charge carriers: $2e^-$ ⇒ 0_{gg} pairs

→ "Gap"

→ $T_c \sim M^{-\alpha}$... isotope effect

⇒ el-ph coupling

Cooper pairs:

$$\psi_0(\vec{r}_1, \vec{r}_2) = \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\vec{r}_1} e^{-i\vec{k}\vec{r}_2}$$

$$\Rightarrow \chi_{SIWC} = \frac{1}{\Omega^2} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Symmetric

$$\Rightarrow \psi_0(\vec{r}_1, \vec{r}_2) = \sum_{\vec{k} > \vec{k}_F} g_{\vec{k}} \cos(\vec{k}(\vec{r}_1 - \vec{r}_2))$$

exercises

$$\Rightarrow SE: V(\vec{r}_1, \vec{r}_2)$$

Fourier space

$$\Rightarrow (E - 2\varepsilon_k) g_k = \sum_{\vec{k}' > \vec{k}_F} V_{kk'} g_{k'}$$

Fourier of $V(\vec{r}_1 - \vec{r}_2)$

• bare Coulomb:

$$V_{k'k} = V_{q=k'-k} = \frac{4\pi^2}{q^2} > 0$$

characterizes
el. screening
↓

- Screening from the electrons:

$$\Rightarrow \text{Thomas-Fermi-Theory: } \mathcal{E}(k) = \frac{k^2 + k_0^2}{k^2}$$

$$\Rightarrow V_q = \frac{4\pi^2}{q^2 + k_0^2} > 0 \quad \dots \text{ smaller than bare Coulomb}$$

- Screening from the nuclei/phonons:

$$\mathcal{E}_{\text{nucl}} = \left(1 + \frac{\omega^2}{\omega^2 - \omega_0^2} \right)$$

$$\Rightarrow \omega = \frac{1}{\hbar} (\mathcal{E}_k - \mathcal{E}_{k'})$$

$$\Rightarrow \left(1 + \frac{\omega^2}{\omega^2 - \omega_q^2} \right) < 0 ?$$

\Rightarrow formally

$$\Rightarrow \omega < \omega_q$$

el-phonon screening can lead to attractive potentials

\vec{c} eigen value \rightarrow $\frac{\partial \mathcal{E}_i(\vec{k})}{\partial \mathcal{U}_5(\vec{q})} \dots$ el-ph-couplings

ph displ. \rightarrow $\left\{ \frac{\partial \mathcal{U}_5(\vec{q})}{\partial \dots} \right\}$

4-index object, not smooth, poles whenever $\mathcal{E}_k - \mathcal{E}_{k+q} = \pm \hbar \omega_0(q)$

$$V_{kk'} = \begin{cases} -V & |\mathcal{E}_k - \mathcal{E}_F|, |\mathcal{E}_{k'} - \mathcal{E}_F| < \hbar \omega_q \\ 0 & \text{else} \end{cases}$$

$$\Rightarrow \frac{1}{V} = \sum_{k > k_F} (2\varepsilon_k - E)^{-1}$$

$$E \approx 2\varepsilon_F - 2\hbar\omega_q e^{-\frac{2}{N V}} < 2\varepsilon_F$$

\Rightarrow Bound state

$N \dots$ number of e^-

$$\psi_0 \sim \frac{V}{2(\varepsilon_k - \varepsilon_F) + 2\varepsilon_F - E} \cos(\vec{k}(\vec{r}_1 - \vec{r}_2))$$

\Rightarrow Bardeen Cooper Schrieffer (BCS)

Main idea: Many-Cooper-pair-WF

$$\psi = \phi(\vec{r}_1 \vec{G}_1, \vec{r}_2 \vec{G}_2) \phi(\dots) \dots \phi(\vec{r}_{N-1} \vec{G}_{N-1}, \vec{r}_N \vec{G}_N)$$

\Rightarrow Hartree-Ansatz | Bosons

$\vec{r}_1, \vec{G}_1 \dots$ ψ has to be antisymmetrized

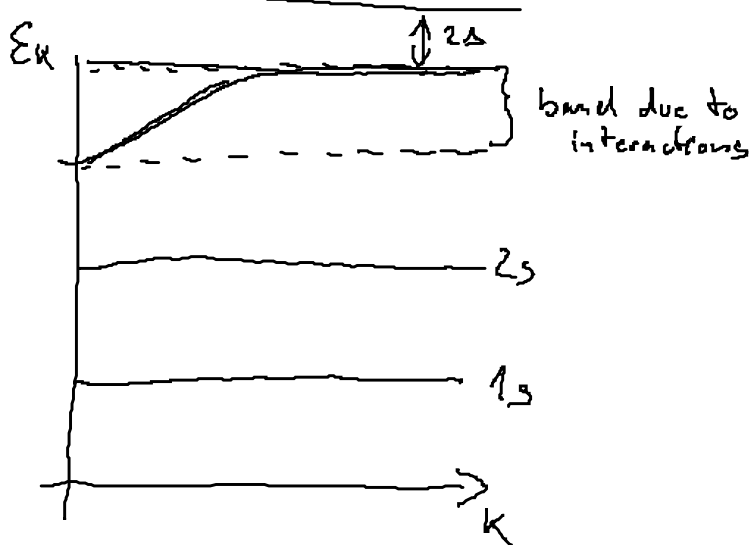
\Rightarrow

$$H = \underbrace{\sum_{\vec{k}, \vec{G}} \varepsilon_k \cdot c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\vec{k}, \vec{k}'} c_{k\uparrow}^\dagger c_{k\downarrow} V_{kk'} c_{-k'\downarrow} c_{k\uparrow}}_{2^{\text{nd}} \text{ quantization}}$$

⇒ Mean-field: Bogoliubov-Transformation

$$H_{MF} = E_0 + \sum_k \epsilon_k \left(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k \right)$$

$$E_0 = 2 \sum_k \left(\epsilon_k V_k + \Delta_k \alpha_k^\dagger \beta_k \right) + \frac{|\Delta|^2}{V}$$



⇒ Conventional SC:

- 2 assumptions: $V_{kk'} \approx \text{constant}$
 $\omega_k \approx \text{material specific}$

⇒ Getting BCS to first principles:

Hardy Gross (FUB, MPI Malle):

- Time dependent DFT for e^-
 - DFT for the nuclei
 - Time dependent DFT for nuclei
- } Bogoliubov-type transformation

first-principle BCS

time-dependent XC functionals
are still inaccurate

→ Metallic Hydrogen should be a SC at room temperature
under pressure

→ H_2S : 1,000,000 bar → $T_c = 203 K$
conventional SC
↳ topic of debate

Unconventional SC:

- e-ph should not be the coupling mechanism
- Cuprates ... AFM effects
→ Magnons
- localized spin-interactions ⇒ Plasmons
- hole-Cooper-pair-formalism

→ Applying theory to a large scale:

- biophysics
- material science problems:
 - defects
 - thermodynamics
- ⇒ LED

→ Developing theories further

- DFT LDA/GGA : decent
- but lot of problems still exist

→ Chemistry / Reactions:
 Non-Equil. Thermodynamics (T, p, μ)

W. Pauli: "Bulks are made by god,
 surfaces by the devil"

⇒ Diamond-like-Carbon / "Gorilla glass"

⇒ Topological Insulators