→ Superconductivity:

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

→ $\chi = -1$ ⇐ defining charact. SC

⇝ charge carriers: $2e^-$ ⇒ Odd pairs

⇝ "Gap"

⇝ $T_c \sim M^{\alpha}$ ... Isotope effect

⇒ el-ph coupling

Cooper pairs:

$$\Psi_0(\vec{r}_1, \vec{r}_2) = \sum_{\vec{k}} g_{\vec{k}} \, e^{i\vec{k}\vec{r}_1} \, e^{-i\vec{k}\vec{r}_2}$$

$$\Rightarrow \chi_{spin} = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

Symmetric

$$\Rightarrow \Psi_0(\vec{r}_1, \vec{r}_2) = \sum_{\vec{k} > \vec{k}_F} g_{\vec{k}}^{s} \cos\left(\vec{k}(\vec{r}_1 - \vec{r}_2)\right)$$

exercises

⇒ SE: $V(\vec{r}_1, \vec{r}_2)$

Fourier space

$$\Rightarrow \left(E - 2\varepsilon_k\right) g_k = \underbrace{\sum_{k' > \vec{k}_F} V_{kk'}}_{\text{Fourier of } V(\vec{r}_1 - \vec{r}_2)} g_{k'}$$

• bare Coulomb:

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

- Screening from the electrons:

characterizes el. screening

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

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

- Screening from the nuclei/phonons:

$$\varepsilon_{nucl} = \left(1 + \frac{\omega^2}{\omega^2 - \omega_0^2}\right)$$

$$\Rightarrow \omega = \frac{1}{\hbar}\left(\varepsilon_k - \varepsilon_{k'}\right)$$

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

$$\Rightarrow \text{formally} \qquad \Rightarrow \omega < \omega_q$$

el-phonon screening can lead to attractive potentials

e^- eigen value

$$\frac{\partial \varepsilon_i(\vec{k})}{\partial u_s(\vec{q})} \quad \ldots \text{ el-ph-couplings}$$

ph displ.

4-index object, not smooth, poles whenever $\varepsilon_k - \varepsilon_{k+q} = \pm\hbar\omega_s(q)$

$$V_{kk'} \approx \begin{cases} -V & |\varepsilon_k - \varepsilon_F|, |\varepsilon_{k'} - \varepsilon_F| < \hbar\omega_q \\ 0 & \text{else} \end{cases}$$

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

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

$\Rightarrow$ Bound state

N ... number of e^-

$$\Psi_0 \sim \frac{V}{2(\varepsilon_k - \varepsilon_F) + 2\varepsilon_F - E} \cos\left(\vec{k}(\vec{r}_1 - \vec{r}_2)\right)$$

$\Rightarrow$ Bardeen Cooper Schrieffer (BCS)

Main idea: Many-Cooper-pair-WF

$$\Psi = \phi(\vec{r}_1 \vec{\sigma}_1, \vec{r}_2 \vec{\sigma}_2)\,\phi(\cdot\ \cdot\cdot)\ \cdots\ \phi(\vec{r}_{N-1} \vec{\sigma}_{N-1}, \vec{r}_N \vec{\sigma}_N)$$

$\Rightarrow$ Hartree-Ansatz | Bosons

$\vec{r}_1, \vec{\sigma}_1$ ... Ψ has to be antisymmetrized

$\Rightarrow$

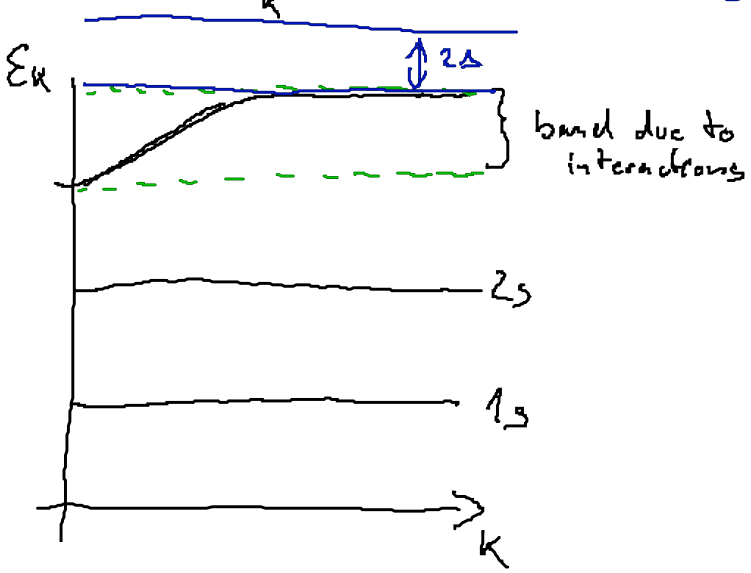
$$H = \sum_{\vec{k},\vec{\sigma}} \varepsilon_k\, c^{+}_{k\sigma} c_{k\sigma} + \sum_{\vec{k}\vec{k}'} c^{+}_{k\uparrow} c^{+}_{-k\downarrow} V_{kk'} c_{-k'\downarrow} c_{k'\uparrow}$$

2nd quantization

⇒ Mean-field: Bogoliubov-Transformation

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

$$E_0 = 2 \sum_k \left(\varepsilon_k v_k + \Delta_k u_k v_k \right) + \frac{|\Delta|^2}{V}$$



⇒ Conventional SC:

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

⇒ Getting BCS to first principles:

Hardy Gross (FUB, MPI Halle):

- ↳ 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 → $T_c = 203K$

conventional SC

↳ topic of debate

Unconventional SC:

- el-ph should not be the coupling mechanism
- Cuprates ... AFM effects
  ⇝ Magnons
- localized spin-interactions ⇒ Plasmons
- hole - Cooper-pair - formalisms

⇒ 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, N)

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

⇝ Diamond-like-Carbon / "Gorilla glas"

⟹ Topological Insulators