Bardeen, Cooper, Schrieffer (BCS) Theory

This Lecture closely follows chapter 6.3 in Ring & Schuck *The nuclear many-body problem*.

BCS ground state:

$$|\mathrm{BCS}\rangle = \prod_{k>0}\left(u_k + v_k \hat{a}_k^\dagger \hat{a}_{\overline{k}}^\dagger\right)|-\rangle$$

$|\overline{k}\rangle$: conjugate state of $|k\rangle$. For time reversal invariant systems, we have $|\overline{k}\rangle = T|k\rangle$, i.e.

$$\begin{aligned} |\overline{n,l,j,j_z}\rangle &= |n,l,j,-j_z\rangle \\ |\overline{\vec{k},\uparrow}\rangle &= |-\vec{k},\downarrow\rangle \end{aligned}$$

BCS state is states where all particles appear in Cooper pairs (i.e. pairs in conjugate orbitals).

Norm of BCS state

$$\langle \mathrm{BCS}|\mathrm{BCS}\rangle = \prod_{k>0}\left(|u_k|^2 + |v_k|^2\right) = 1 \quad \longrightarrow \quad |u_k|^2 + |v_k|^2 = 1.$$

BCS state does not exhibit a fixed particle number:

$$\begin{aligned} \langle N\rangle = \langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle &= 2\sum_{k>0} v_k^2 \\ \langle \mathrm{BCS}|\hat{N}^2|\mathrm{BCS}\rangle - \langle N\rangle^2 &= 4\sum_{k>0} u_k^2 v_k^2 \end{aligned}$$

BCS equations

Two-body Hamiltonian

$$H = \sum_{k,l\neq 0} t_{kl}\hat{a}_k^\dagger \hat{a}_l + \frac{1}{4}\sum_{ijkl} \overline{v}_{ijkl}\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

Particle number fixed by Lagrange multiplier μ (chemical potential) via $H' = H - \mu N$.

Energy expectation value:

$$\begin{aligned} E = \langle \mathrm{BCS}|H'|\mathrm{BCS} &= \sum_{k\neq 0}\left((t_{kk}-\mu)v_k^2 + \frac{1}{2}\sum_l \overline{v}_{klkl} v_k^2 v_l^2\right) \\ &+ \sum_{k,l>0} \overline{v}_{k\overline{k}l\overline{l}} u_k v_k u_l v_l \end{aligned}$$

Variation of energy (use $u_k^2 + v_k^2 = 1 \to \partial u_k/\partial v_k = -v_k/u_k$)

$$0 = \frac{d}{dv_k}E = \left(\frac{\partial u_k}{\partial v_k} + \frac{\partial}{\partial u_k}\right) E$$

yields

$$\begin{aligned} 0 &= 2\tilde{\varepsilon}_k u_k v_k + \Delta_k (v_k^2 - u_k^2) && (1) \\ \tilde{\varepsilon}_k &\equiv \frac{1}{2}\left(t_{kk} + t_{\overline{k},\overline{k}} + \sum_{l\neq 0}\left(\overline{v}_{klkl} + \overline{v}_{\overline{k}l\overline{k}l}\right) v_l^2\right) - \mu && (2) \\ \Delta_k &\equiv -\sum_{l>0} \overline{v}_{k\overline{k}l\overline{l}} u_l v_l && (3) \end{aligned}$$

One can solve the first of these three equations for the occupation numbers and finds

$$\begin{aligned} v_k^2 &= \frac{1}{2}\left(1 - \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\right) \\ u_k^2 &= \frac{1}{2}\left(1 + \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\right) \end{aligned}$$

Recall that v_k^2 is the occupation probability for state k. Thus, the pairing interaction destabilizes the Fermi surface!

Inserting these results into Eq. (1) yields the *Gap Equation*

$$\Delta_k = -\frac{1}{2}\sum_{l>0} \overline{v}_{k\bar{k}l\bar{l}} \frac{\Delta_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}$$

This equation, together with the Equation for the energies $\tilde{\varepsilon}_k$ has to be solved iteratively.

Simple examples and illustration:

(1) Pure pairing force: $\overline{v}_{ijkl} = -G, \quad t_{k,l} = \delta_{kl}\varepsilon_l$
Gap equation

$$\Delta = \frac{G}{2}\sum_{l>0} \frac{\Delta}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta_k^2}}$$

For vanishing single-particle energies $\varepsilon_k = 0$ and a single-j shell one recovers the results of the seniority model. The gap becomes

$$\Delta = G\sqrt{\frac{n}{2}\left(\Omega - \frac{N}{2}\right)} = \frac{G\Omega}{2}$$

at half filling. Comparison with the seniority model shows that 2Δ is the energy to break a pair and equals the excitation energy!

(2) Analytical solution for simple model.

Assume constant interaction G, constant gap Δ, and constant density of states ρ, and restrict summation to the vicinity δ of the Fermi surface. Gap equation:

$$1 = \frac{G}{2} \int_{\mu-\delta}^{\mu+\delta} d\varepsilon \frac{\rho(\varepsilon)}{\sqrt{(\varepsilon-\mu)^2 + \Delta^2}} = G\rho \; \mathrm{arsinh} \frac{\delta}{\Delta}$$

For weak pairing $G\rho \ll 1$ one finds

$$\frac{\Delta}{\delta} \propto \exp\left(\frac{-1}{|G|\rho}\right)$$

Gap is nonperturbative in interaction G!

The particle number variance is

$$(\Delta N)^2 \approx 2\rho\Delta \; \mathrm{atan} \frac{\delta}{\Delta} = \begin{cases} \pi\rho\Delta & \text{for weak pairing } \Delta \ll \delta, \\ 2\rho\delta & \text{for strong pairing.} \end{cases}$$

BCS essentials

1. The Fermi surface of a Fermi gas is unstable with respect to *attractive* interactions. The gap equation has a nontrivial solution $\Delta \neq 0$ whenever the interaction or the density of states is sufficiently large.

2. The finite excitation gap causes superfluidity: The system cannot absorb arbitrarily small perturbations and therefore remains inert (See, e.g., Landau & Lifshitz, Statistical Mechanics II).

Bogoliubov quasi-particles

The BCS state can also be written as

$$|\mathrm{BCS}\rangle \propto \prod_{k\neq 0} \hat{\alpha}_k |-\rangle$$

where we used the *quasi-particle* operators

$$\begin{aligned}\hat{\alpha}_k^\dagger &= u_k \hat{a}_k^\dagger - v_k \hat{a}_{\overline{k}},\\ \hat{\alpha}_{\overline{k}}^\dagger &= u_k \hat{a}_{\overline{k}}^\dagger + v_k \hat{a}_k.\end{aligned}$$

The quasi-particle operators fulfill the canonical anti-commutation rules since $|u_k|^2 + |v_k|^2 = 1$.

One has $\hat{\alpha}_k|\mathrm{BCS}\rangle = 0$.

The BCS state of an interacting system is thus a simple product state of non-interacting quasi-particles! The price tag consists of the non-conservation of particle number. This approach is fruitful as it allows to define excited states in terms of quasi-particle excitations.