

BEHAVIOR AT NON-ZERO T:THE BOGOLIUBOV-DE GENNES FORMALISM

- The BdG approach seeks to solve the BCS pairing Hamiltonian

$$\mathcal{H} = \sum_{k,\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma} V_{kk} c_{k\sigma}^\dagger c_{-k\sigma}^\dagger c_{-k\sigma} c_{k\sigma} \quad (1)$$

by mean-field decoupling:

$$c_{k\sigma}^\dagger c_{-k\sigma}^\dagger c_{-k\sigma} c_{k\sigma} \rightarrow c_{k\sigma}^\dagger c_{-k\sigma}^\dagger \langle c_{-k\sigma} c_{k\sigma} \rangle + \langle c_{k\sigma}^\dagger c_{-k\sigma}^\dagger \rangle c_{-k\sigma} c_{k\sigma} - \langle \dots \rangle \langle \dots \rangle \quad (2)$$

Now define a "pairing field"

$$\Delta_k = \sum_\sigma V_{kk} \langle c_{-k\sigma} c_{k\sigma} \rangle \quad (3)$$

The Hamiltonian (1) can be approximated by

$$\left[\mathcal{H}_{BdG} = \sum_{k,\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k \left(\Delta_k c_{k\sigma}^\dagger c_{k\sigma}^+ + \Delta_k^* c_{-k\sigma}^\dagger c_{-k\sigma} \right) - \sum_k \Delta_k \langle c_{k\sigma}^\dagger c_{-k\sigma}^\dagger \rangle \right] \quad (4)$$

This is the mean-field BdG Hamiltonian which we can diagonalize by means of a canonical transformation.

- Define a "Nambu spinor"

$$\psi_k = \begin{pmatrix} c_{k\sigma} \\ c_{-k\sigma}^\dagger \end{pmatrix} \quad (5)$$

and write

$$\left[\mathcal{H}_{BdG} = \sum_k \psi_k^\dagger \underbrace{\begin{pmatrix} \xi_k & \Delta_k \\ \Delta_k^* & -\xi_k \end{pmatrix}}_{h_k} \psi_k + E_0 \right] \quad (6)$$

$$E_0 = \sum_k \xi_k - \sum_k \Delta_k \langle c_{k\sigma}^\dagger c_{-k\sigma}^\dagger \rangle$$

- The 2×2 matrix has eigenvalues $\pm E_k$ where

$$E_k = \sqrt{\xi_k^2 + \Delta_k^2} \quad (7)$$

In the diagonal basis the BdG Hamiltonian (6) can be re-cast as

$$\boxed{H_{\text{BdG}} = \sum_k E_k (\gamma_{k1}^+ \gamma_{k1} - \gamma_{k2}^+ \gamma_{k2}) + E_0} \quad (8)$$

where $\gamma_{k\sigma}$ are BdG quasiparticle operators related to $c_{k\sigma}$ by a unitary transformation $(\gamma_{k1} \gamma_{k2}) = U_k \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^+ \end{pmatrix}$ where U_k diagonalizes the (2×2) h_k matrix in (6).

- The ground state: We see that because $E_k \geq 0$ the g.s. of Hamiltonian (8) consists of all γ_{k2} states OCCUPIED and all γ_{k1} states empty:

$$|\Psi_0\rangle = \prod_k \gamma_{k2}^+ |\text{0}\rangle \quad (9)$$

- Excitations: - We can add γ_{k1} particle (or remove γ_{k2}) which costs energy E_k . This implies E_k is the spectrum of excitations.

- Whenever $\min_k \Delta_k > 0$ the excitation spectrum is GAPPED - true in most but not all superc.

- Hence, Δ_k is often called "SC gap function"

- Connection to the BCS wave function: It is easy to check that (u_k) and (v_k^*) are eigenstates of 2×2 matrix h_k with eigenvalues $\pm \sqrt{\xi_k^2 + \Delta_k^2}$, hence $U_k = \begin{pmatrix} u_k & v_k^* \\ v_k & -u_k^* \end{pmatrix}$.

• Calculation of Δ and the critical temperature T_c

- We determine Δ at non-zero temperature by minimizing the system free energy $F = -\frac{1}{\beta} \ln Z$ where Z is the partition function

$$Z = \sum_{\{n\}} e^{-\beta E\{n\}} \quad (10)$$

Here $E\{n\} = \sum_k n_{k1} E_k - \sum_k n_{k2} E_k + E_0$ and $n_{k\alpha} = 0, 1$

denote occupation numbers of two fermions.

$$Z = \sum_{n_{k1}, n_{k2}} e^{-\beta \sum_k E_k n_{k1}} e^{\beta \sum_k E_k n_{k2}} e^{-\beta E_0} \quad (11)$$

$$= e^{-\beta E_0} \prod_k (1 + e^{-\beta E_k}) (1 + e^{\beta E_k})$$

$$= e^{-\beta E_0} \prod_k (e^{\frac{1}{2}\beta E_k} + e^{-\frac{1}{2}\beta E_k})^2 = e^{-\beta E_0} \prod_k 4 \cosh^2 \frac{1}{2} \beta E_k$$

$$\Rightarrow F = E_0 - \frac{1}{\beta} \sum_k 2 \ln(2 \cosh \frac{1}{2} \beta E_k) \quad (12)$$

- Recall that $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ and $E_0 = \sum_k \xi_k - \sum_k \Delta_k \langle c_{k\downarrow}^\dagger c_{k\downarrow} \rangle$.

Once again we adopt the Cooper ansatz for V_{ee} :

$$\Delta_k = \begin{cases} \Delta = -V \sum_\ell \langle c_{e\downarrow\ell} c_{e\uparrow\ell} \rangle, & |\xi_\ell| < \hbar w, \\ 0, & \text{otherwise} \end{cases}$$

$$\text{Then } E_0 = \sum_k \xi_k + \frac{1}{V} \Delta^2 \quad (13)$$

• Minimize the free energy:

$$\frac{\partial F}{\partial \Delta} = +\frac{2}{V} \Delta - 2 \sum_k \frac{\partial E_k}{\partial \Delta} \tanh \frac{1}{2} \beta E_k \quad (14)$$

$$\frac{\partial E_k}{\partial \Delta} = \frac{\Delta}{\sqrt{\xi_k^2 + \Delta^2}} = \frac{\Delta}{E_k}$$

$$\boxed{\frac{\Delta}{V} = \frac{1}{2} \sum_k' \frac{\Delta}{E_k} \tanh \frac{1}{2} \beta E_k} \quad (15)$$

↑ "BCS gap equation" at nonzero T

- At $T=0$ this becomes

$$\frac{\Delta}{V} = \frac{1}{2} \sum_k' \frac{\Delta}{E_k} \quad - \text{we already solved this to obtain}$$

$$\boxed{\Delta \approx 2\pi w_c e^{-1/N(0)V}} \quad (\text{the BCS result}) \quad (16)$$

- At $T>0$ Eq. (15) must be solved by numerical iteration,

one obtains $\Delta(T) \rightarrow \Delta(T)$

- the critical temperature T_c

can be obtained as follows:

As $T \rightarrow T_c$ we have

$\Delta(T) \rightarrow 0$ and hence

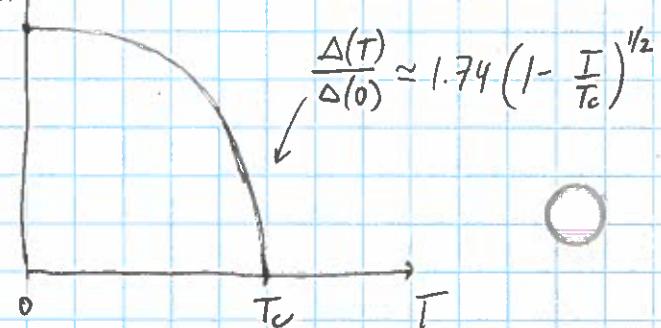
$E_k \rightarrow |\zeta_k|$. We thus replace in (15) E_k by $|\zeta_k|$ and solve:

$$\frac{1}{V} = \frac{1}{2} \sum_k' \frac{1}{|\zeta_k|} \tanh \frac{1}{2} \beta |\zeta_k| \quad (17)$$

$$\begin{aligned} \rightarrow \frac{1}{V} &= N(0) \int_0^{\pi w_c} d\xi \frac{1}{\xi} \tanh \frac{1}{2} \beta \xi \\ &= N(0) \int_0^{\beta \pi w_c / k_B T} dx \frac{\tanh x}{x} \\ &= N(0) \ln \left(\frac{2\gamma}{\pi} \beta c \pi w_c \right) \end{aligned} \quad (18)$$

Here γ is Euler's constant and $2\gamma/\pi \approx 1.13$.

$$\Rightarrow \boxed{k_B T_c = \frac{1}{\beta c} = 1.13 \pi w_c e^{-1/N(0)V}} \quad (19)$$



• BCS universal ratio: Dividing Eq. (19) by (16) we find

$$\frac{\Delta(0)}{k_B T_c} = \frac{2}{1.13} = 1.76 \quad (20)$$

Both $\Delta(0)$ and T_c are measurable. One finds experimental values of $\Delta(0)/k_B T_c$ to range between 1.5 - 2.3 in most superconductors, in agreement with the prediction of BCS.

- Thermodynamic properties:

Calculation of the specific heat

- Specific heat of electrons in a superconductor is most easily obtained from entropy using thermodynamic identity

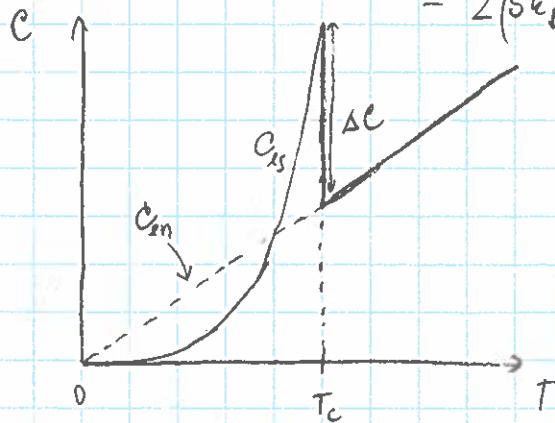
$$C_{es} = T \frac{dS_{es}}{dT} = -\beta \frac{dS_{es}}{d\beta} \quad (21)$$

Here S_{es} denotes entropy of the fermion gas Eq. (8).

$$S_{es} = -2k_B \sum_k \left[(1-n_k) \ln (1-n_k) + n_k \ln n_k \right] \quad (22)$$

Evaluate:

$$\begin{aligned} C_{es} &= 2\beta k_B \sum_k \frac{\partial n_k}{\partial \beta} \ln \frac{n_k}{1-n_k} = -2\beta^2 k_B \sum_k E_k \frac{\partial n_k}{\partial \beta} \\ &= -2\beta^2 k_B \sum_k E_k \frac{d n_k}{d(\beta E_k)} \left(E_k + \beta \frac{d E_k}{d \beta} \right) \\ &= 2\beta k_B \sum_k \left(-\frac{\partial n_k}{\partial E_k} \right) \left(E_k + \frac{1}{2}\beta \frac{d E_k}{d \beta} \right) \end{aligned} \quad (23)$$



- The SC transition at T_c is marked by a JUMP in C whose size ΔC can be calculated as

$$\frac{\Delta C}{C_{en}} \approx 1.43 \quad (24)$$