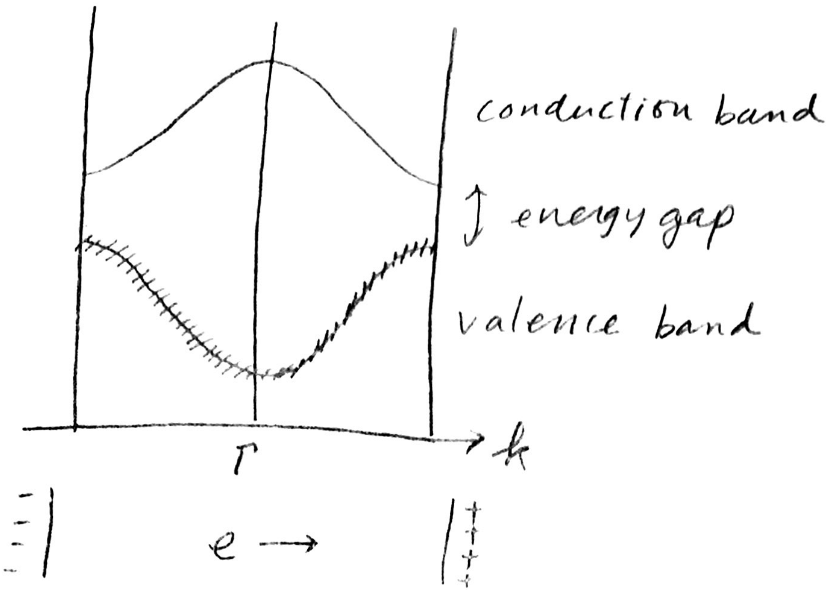
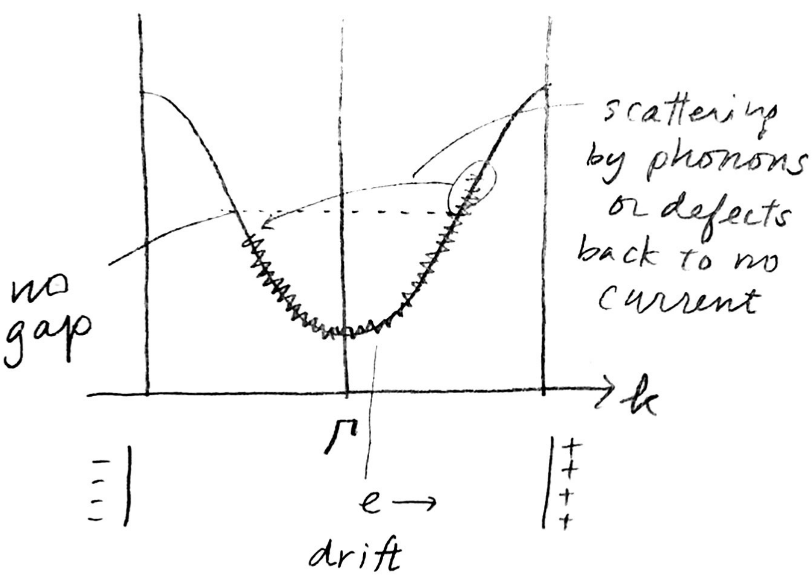
① Insulator, normal conductor, and superconductor



ⓐ Insulator

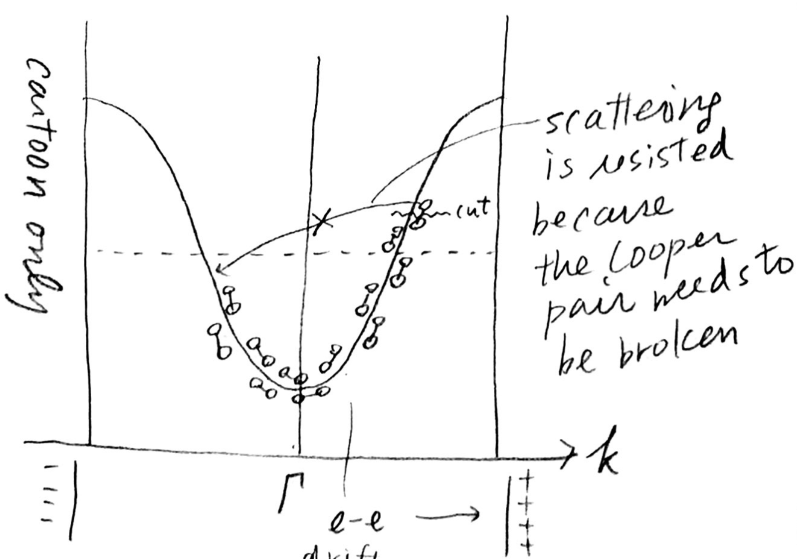
When voltage is applied, electrons want to accelerate, but the gap prevents it

— no current; insulator



ⓑ Normal conductor

With no gap, electrons can have drift velocities and current. Scattering will bring the high-velocity electrons back to lower velocities.



ⓒ Superconductor

The superconducting gap "moves" with electron pairs, so there's current. Scattering is resisted because the Cooper pair needs to be broken (or the SC gap must be overcome)

No Ohmic resistence.

② Meissner effect (perfect diamagnetism) is implied by perfect conductivity

London's equations

superconducting current

$$\mathbb{E} = \frac{\partial}{\partial t}(\Lambda \mathbb{J}) \qquad \text{①}$$

electric field

phenomenological parameter

current increases endlessly when a field is applied (unlike in a normal conductor a current is merely sustained by a field)

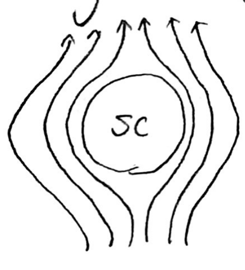
$$\nabla \times (\Lambda \mathbb{J}) = -\mathbb{B} \qquad \text{②}$$

magnetic field

Combining ② with Maxwell's eq. $\nabla \times \mathbb{B} = \mu_0 \mathbb{J}$

$$\nabla \times \left(\nabla \times \frac{\Lambda}{\mu_0} \mathbb{B}\right) = -\mathbb{B}$$

Using $\nabla \times (\nabla \times \mathbb{X}) = \nabla(\nabla \cdot \mathbb{X}) - \nabla^2 \mathbb{X}$ and $\nabla \cdot \mathbb{B} = 0$ (Maxwell eq)



$$\nabla^2 \mathbb{B} = \frac{\mathbb{B}}{\lambda^2}$$

meaning $\mathbb{B}$ exponentially decays inside a SC - Meissner effect

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Derivation of ① and ②

$$\mathbb{J} = n_s e v \;; \quad m\frac{\partial v}{\partial t} = e\mathbb{E} \longrightarrow \mathbb{E} = \frac{\partial}{\partial t}\left(\frac{m}{n_s e^2} J\right)$$

electrons

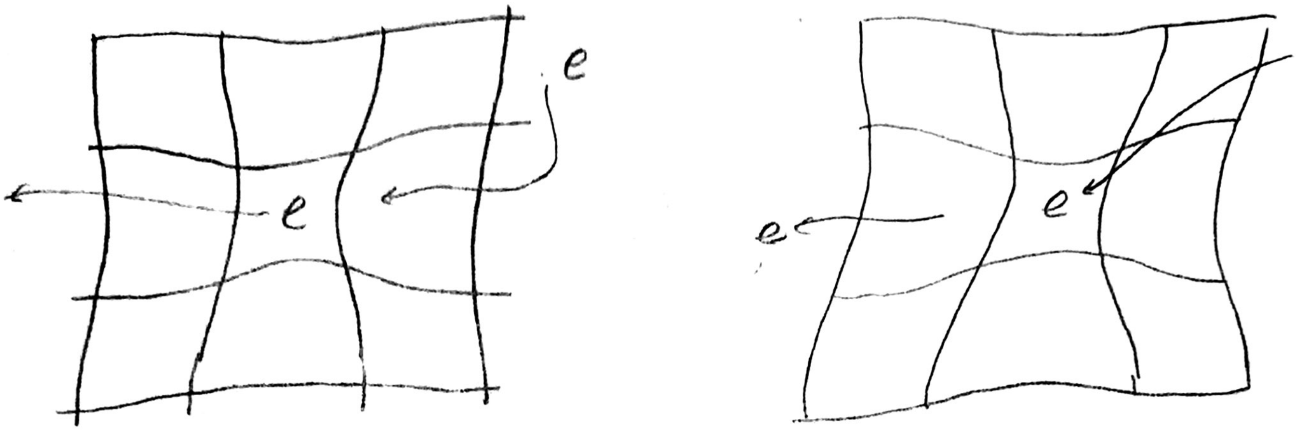
Newton eq.

Λ

Taking $\nabla \times$ $\quad \nabla \times \mathbb{E} = \frac{\partial}{\partial t}(\nabla \times \Lambda \mathbb{J}) \;; \quad \nabla \times \mathbb{E} = -\frac{\partial \mathbb{B}}{\partial t}$ (Maxwell) $\rightarrow \nabla \times (\Lambda \mathbb{J}) = -\mathbb{B}$

③ Superconductivity theory outline

1) Fröhlich's theory of attractive electron-electron interaction through lattice vibration



2) Cooper's theory of electron pair formation

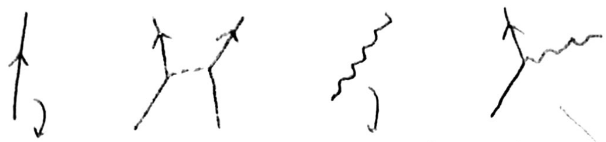
3) BCS theory of superconducting gap and a near universal relationship $\frac{2\Delta}{kT_c} = 3.52$

superconducting transition temperature

④ Fröhlich's theory (Mattuck, p. 257)

The bare Hamiltonian of a superconductor is

$$\hat{H} = \hat{H}_e + \hat{H}_{e-e} + \hat{H}_{ph} + \hat{H}_{e-ph}$$



$\sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$ $\sum \Omega_q (B_q^\dagger B_q + \frac{1}{2})$

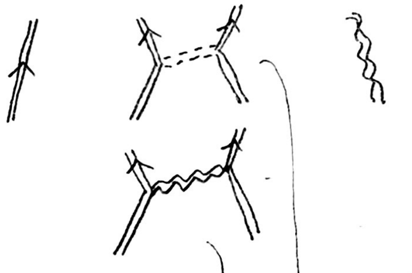
$\frac{1}{2} \sum V_K \, c^\dagger_{k'-K,\sigma'} c^\dagger_{k+K,\sigma} c_{k\sigma} c_{k'\sigma'}$ $\sum g_q [B_q + B^\dagger_{-q}] c^\dagger_{k'\sigma} c_{k\sigma}$

$V_K \to 4\pi/K^2$

What we want to know is the effective e-e interaction mediated by phonons

Fröhlich showed that by a series of canonical transformations the above $\hat{H}$ can be transformed into

$$\hat{H} = \hat{H}'_e + \hat{H}'_{e-e} + \hat{H}'_{ph} \quad (+ \text{ no more bare } \hat{H}_{e-ph}!)$$



$\sum_{k,\sigma} \epsilon'_k c^\dagger_{k\sigma} c_{k\sigma}$ $\sum \omega_q (B_q^\dagger B_q + \frac{1}{2})$

$$\frac{1}{2} \sum V'_{kq} \, c^\dagger_{k'-q,\sigma'} c^\dagger_{k+q,\sigma} c_{k\sigma} c_{k'\sigma'}$$

$$V'_{kq} = \frac{4\pi}{q^2+\lambda^2} + \frac{2\omega_q |g_q|^2}{(\epsilon_k - \epsilon_{k+q})^2 - \omega_q^2} \leftarrow ※$$

screened Coulomb e-ph-e interaction

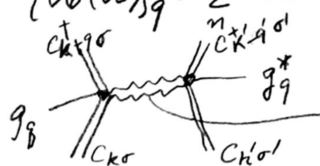
Note:

Coulomb $\frac{1}{r} \xleftrightarrow{FT} \frac{4\pi}{k^2}$

Yukawa $\frac{e^{-\lambda r}}{r} \xleftrightarrow{FT} \frac{4\pi}{k^2+\lambda^2}$

Perhaps an easier way to see how this expression emerges is each line in a diagram is 0^{th} Green's fxn. (Hermes, Hirata, JCP 139, 034111, (2013))

$$\{G_0(\omega)\}_q = \sum_n \frac{\langle 0|B_q + B^\dagger_{-q}|n\rangle\langle n|B^\dagger_q + B_{-q}|0\rangle}{\omega - (E_n^{(0)} - E_0^{(0)}) + i\delta} + \sum_n \frac{\langle 0|B^\dagger_q + B_{-q}|n\rangle\langle n|B_q + B^\dagger_{-q}|0\rangle}{-\omega - (E_n^{(0)} - E_0^{(0)}) + i\delta} = \frac{2\omega_q}{\omega^2 - \omega_q^2}$$

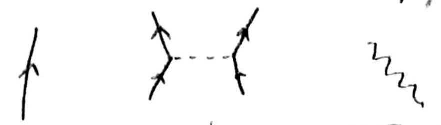


$\frac{2\omega_q}{\omega^2 - \omega_q^2}$; $\omega = \epsilon_{k+q} - \epsilon_k$

Important: ※ can be negative (e-ph-e attractive) when $|\epsilon_k - \epsilon_{k+q}| < \omega_q$

④′ Fröhlich's theory redux (Kittel "Quantum Theory of Solids" 2^{nd} Ed. p. 151)

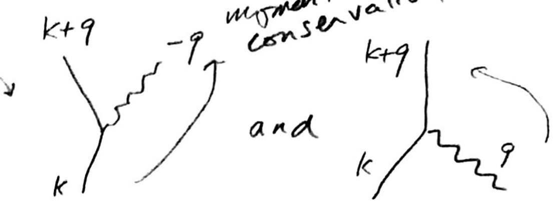
$$\hat{H} = \underbrace{\hat{H}_e + \hat{H}_{e-e} + \hat{H}_{ph}}_{\hat{H}_0} + \hat{H}_{e-ph}$$



$\sum_k \epsilon_k C_k^{\dagger} C_k$ $\quad$ $\sum \Omega_q (B_q^{\dagger} B_q + \frac{1}{2})$

$\frac{1}{2} \sum V_K C_{K'-K}^{\dagger} C_{K+K}^{\dagger} C_K C_{K'}$

Coulomb



$$\underbrace{\sum g_q C_{k+q}^{\dagger} C_k B_{-q}^{\dagger} \quad \sum g_q C_{k+q}^{\dagger} C_k B_q}_{\lambda \hat{H}'}$$

We want to canonical transform $\bar{H} = e^{-S}\hat{H}e^{S} = e^{-\lambda S}(\hat{H}_0 + \lambda \hat{H}')e^{\lambda S}$ has no term proportional to λ; $\bar{H}$ will be (cf. coupled-cluster theory)

$\bar{H} =$

effective e-e interaction via phonon

In other words, we partially diagonalize $\hat{H} \to \bar{H}$, so off-diagonal elements linear in g (or λ) are made to vanish.

$$(1)\quad e^{-S}\hat{H}e^{S} = (1 - S + \frac{S^2}{2} + \cdots)\hat{H}(1 + S + \frac{S^2}{2} + \cdots)$$

$$= \hat{H} + \hat{H}S - S\hat{H} + \tfrac{1}{2}(\hat{H}S^2 - 2S\hat{H}S + S^2\hat{H}) + \cdots$$

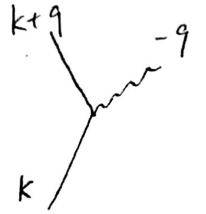
$$= \hat{H} + [\hat{H}, S] + \tfrac{1}{2}[[\hat{H}, S], S] + \cdots \quad \text{Hausdorff expansion}$$

$$(2)\quad e^{-\lambda S}(\hat{H}_0 + \lambda\hat{H}')e^{\lambda S} = \hat{H}_0 + \underbrace{\lambda\hat{H}' + \lambda[\hat{H}_0, S]}_{\text{linear in } \lambda} + \lambda^2[\hat{H}', S] + \frac{\lambda^2}{2}[[\hat{H}_0, S], S] \cdot$$

(3) $\hat{H}' + [\hat{H}_0, S] = 0$ determines S that partially diagonalizes $\hat{H}$

$$(4)\quad \underbrace{\langle n|}_{\text{eigenfxns of } \hat{H}_0} H'|m\rangle + \underbrace{\langle n|\hat{H}_0}_{E_n\langle n|} S|m\rangle - \langle n|S\underbrace{\hat{H}_0|m\rangle}_{E_m|m\rangle} = 0 \to \langle n|S|m\rangle = \frac{\langle n|\hat{H}'|m\rangle}{E_m - E_n}$$

(5)



$|n\rangle = |k+q, \omega_{-q}\rangle$

$E_n = \varepsilon_{k+q} + \omega_{-q}$

$E_m = \varepsilon_k$

$|m\rangle = |k, 0\rangle$

↑ e. state ↑ phonon state

$|n\rangle = |k+q, 0\rangle$

$E_n = \varepsilon_{k+q}$

$E_m = \varepsilon_k + \omega_q$

$|m\rangle = |k, \omega_q\rangle$

$$\hat{H}' = \Sigma\, g_q\, C^\dagger_{k+q} C_k B^\dagger_{-q} \quad + \quad \Sigma\, g_q\, C^\dagger_{k+q} C_k B_q$$

$$\langle n|S|m\rangle = \frac{\langle n|\hat{H}'|m\rangle}{E_m - E_n} = \frac{g_q}{\varepsilon_k - \varepsilon_{k+q} - \omega_{-q}}$$

$$\langle n|S|m\rangle = \frac{\langle n|\hat{H}'|m\rangle}{E_m - E_n} = \frac{g_q}{\varepsilon_k - \varepsilon_{k+q} + \omega_q}$$

(6) With these S,

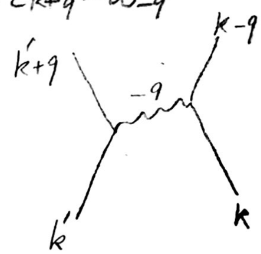
$$\bar{H} = \hat{H}_0 + \lambda\underbrace{\left(\hat{H}' + [\hat{H}_0, S]\right)}_{\to 0} + \lambda^2\left([\hat{H}', S] + \frac{1}{2}[\underbrace{[\hat{H}_0, S]}_{-\hat{H}'}, S]\right) + \cdots$$

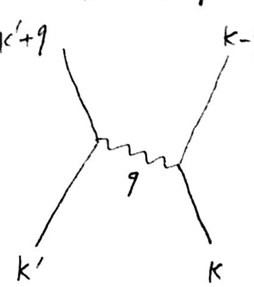
$$= \hat{H}_0 + \frac{\lambda^2}{2}[\hat{H}', S] + O(\lambda^3)$$

sum over m, n, m'

(7)
$$\frac{1}{2}[\hat{H}', S] = \frac{1}{2}\left(|m\rangle\langle m|H'|n\rangle\langle n|S|m'\rangle\langle m'|\right) - \frac{1}{2}\left(|m\rangle\langle m|S|n\rangle\langle n|H'|m'\rangle\langle m'|\right)$$

$$= \frac{|g_q|^2}{2}\frac{C^\dagger_{k-q} C_k C^\dagger_{k'+q} C_{k'}}{\varepsilon_k - \varepsilon_{k+q} - \omega_{-q}} - \frac{|g_q|^2}{2}\frac{C^\dagger_{k-q} C_k C^\dagger_{k'+q} C_{k'}}{\varepsilon_k - \varepsilon_{k+q} + \omega_q}$$



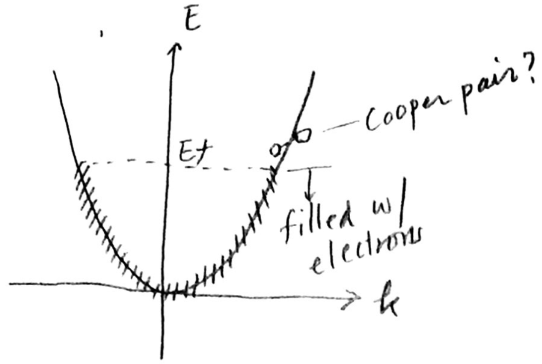


$$= \frac{|g_q|^2}{2}\frac{2\omega_q}{(\varepsilon_k - \varepsilon_{k+q})^2 - \omega_q^2}$$

$(\because \omega_q = \omega_{-q})$

$$= \frac{\omega_q |g_q|^2}{(\epsilon_k - \varepsilon_{k+q})^2 - \omega_q^2} \quad \text{e-ph-e interaction}$$

⑤ Cooper pair formation (March, p. 219 ; Mattuck, p. 260)



$$\Big(-\frac{1}{2}\nabla_1^2-\frac{1}{2}\nabla_2^2+\underbrace{v(\mathbf{r}_1,\mathbf{r}_2)}_{\substack{\text{Fröhlich}\\ e\text{-}e\text{ attractive}\\ \text{potential}}}\Big)\psi = E\psi \quad \text{— ①}$$

Q: When $v=0$, $E = E_f$. When $v<0$, will the lowest energy of a pair consisting of unoccupied orbitals ($k>k_f$) be lower than E_f ?

A: $\psi = \sum_{k>k_f} C_{\mathbf{k}}\, e^{i\mathbf{k}\cdot\mathbf{r}_1}\cdot e^{i(-\mathbf{k})\cdot\mathbf{r}_2}$ ← pairing of $\mathbf{k}$ and $-\mathbf{k}$ (ignoring spins for simplicity) (setting unit cell volume = 1)

$k>k_f$ — electrons are in unoccupied orbitals

Substituting in ①

$$\sum_{k>k_f} C_{\mathbf{k}}\Big(\underbrace{\frac{|\mathbf{k}|^2}{2}+\frac{|\mathbf{k}|^2}{2}}_{E_k}-E+v(\mathbf{r}_1,\mathbf{r}_2)\Big)\, e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$$

Multiplying w/ $e^{-i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)}$ and integrating over $\mathbf{r}_1$ and $\mathbf{r}_2$

$$(E_{k'}-E)\,C_{\mathbf{k}'} = -\sum_{k>k_f} C_{\mathbf{k}}\,\underbrace{v(\mathbf{k}',-\mathbf{k}',\mathbf{k},-\mathbf{k})}_{\iint e^{-i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)}\, v\, e^{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)}\,d\mathbf{r}_1 d\mathbf{r}_2}$$

Assuming

$$v(\mathbf{k}',-\mathbf{k}',\mathbf{k},-\mathbf{k}) = \begin{cases} -v & E_f < E_k,\ E_{k'} < E_f+\delta \\ 0 & \end{cases}$$

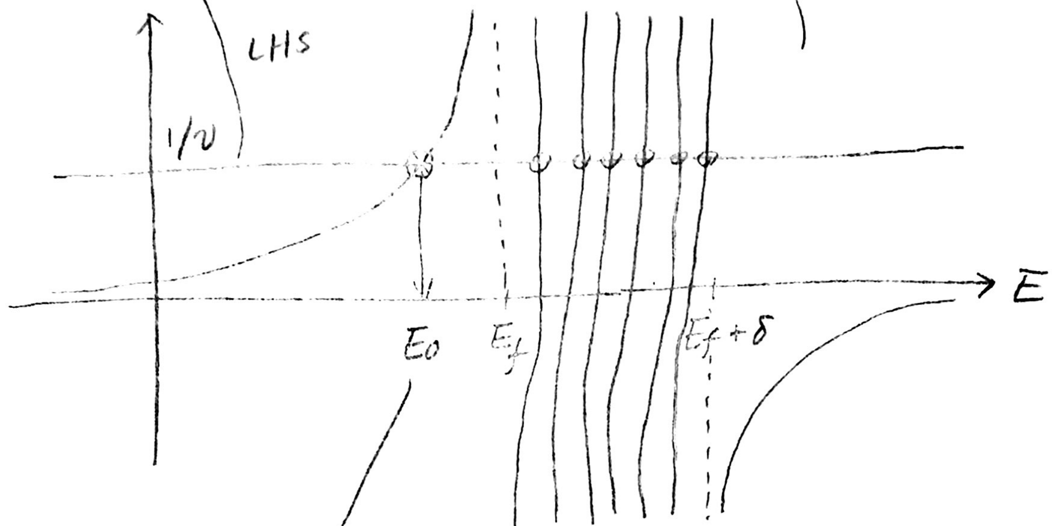
$$C_{\mathbf{k}'} = \frac{v}{E_k'-E}\sum_{E_f<E_k<E_f+\delta} C_{\mathbf{k}}$$

Summing over E_k' $\longrightarrow$ cancel

$$\sum_{E_f < E_k' < E_f+\delta} C_{k'} = \sum_{E_f < E_k' < E_f+\delta} \frac{v}{E_k' - E} \sum_{E_f < E_k < E_f+\delta} C_k$$

$$\frac{1}{v} = \sum_{E_f < E_k' < E_f+\delta} \frac{1}{E_k' - E} \quad \leftarrow \text{RHS}$$

LHS



Stable Cooper pair energy $E_0 < E_f$

In a matrix view, consider 2 electrons in 6 states near Fermi surface

$|k_1\uparrow \quad -|k_1\downarrow \qquad |k_2\uparrow \quad -|k_2\downarrow \qquad |k_3\uparrow \quad -|k_3\downarrow$

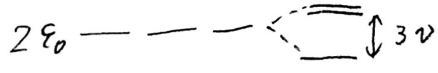
Three pair basis functions

$\|1\rangle$	⊖ ⊖	— —	— —	$2\varepsilon_0$
$\|2\rangle$	— —	⊖ ⊖	— —	$2\varepsilon_0$
$\|3\rangle$	— —	— —	⊖ ⊖	$2\varepsilon_0$

Same $v(|k', -|k', |k, -|k) = -v$ (near Fermi surface)

$$\hat{H} = \begin{pmatrix} 2\varepsilon_0 & 0 & 0 \\ 0 & 2\varepsilon_0 & 0 \\ 0 & 0 & 2\varepsilon_0 \end{pmatrix} - \begin{pmatrix} 0 & v & v \\ v & 0 & v \\ v & v & 0 \end{pmatrix} \longrightarrow \text{eigenvalues are}$$

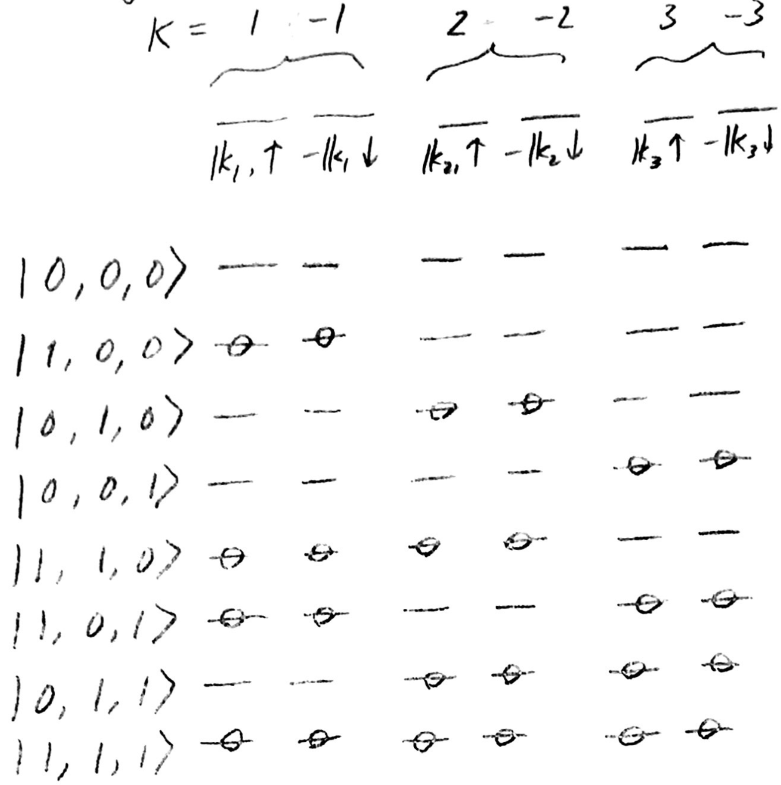
$2\varepsilon_0 + v,\ 2\varepsilon_0 + v,\ 2\varepsilon_0 \underline{-2v}$



stable Cooper pair $< 2\varepsilon_0$

⑥ Bardeen - Cooper - Schrieffer theory

We want to generalize the last page's model to many electrons



$$|\Psi_{sc}\rangle \equiv \prod_K (u_K + v_K \hat{a}_K^\dagger \hat{a}_{-K}^\dagger)|0\rangle$$

$u_1 u_2 u_3 \; |000\rangle$

$v_1 u_2 u_3 \; |100\rangle$

$u_1 v_2 u_3 \; |010\rangle$

$u_1 u_2 v_3 \; |001\rangle$

$v_1 v_2 u_3 \; |110\rangle$

$v_1 u_2 v_3 \; |101\rangle$

$u_1 v_2 v_3 \; |011\rangle$

$v_1 v_2 v_3 \; |111\rangle$

- We want to show that $|\Psi_{sc}\rangle$ parametrized as such has a lower energy than the ground state upon turning on the attractive e-e interaction.
- We also want to show that the smallest excitation energy, breaking a Cooper pairing, is nonzero, causing the SC gap.

Normalization:

$$1 = \langle \Psi_{sc} | \Psi_{sc} \rangle = u_1^2 u_2^2 u_3^2 + v_1^2 u_2^2 u_3^2 + \cdots + v_1^2 v_2^2 v_3^2$$

$$= (u_1^2 + v_1^2)(u_2^2 + v_2^2)(u_3^2 + v_3^2)$$

We demand $u_K^2 + v_K^2 = 1$

The expectation value of the number of electrons:

$$\langle \Psi_{sc} | \hat{N} | \Psi_{sc} \rangle = 0 \cdot u_1^2 u_2^2 u_3^2 + 2 \cdot v_1^2 u_2^2 u_3^2 + \cdots + 6 \cdot v_1^2 v_2^2 v_3^2$$

$$= 2 (v_1^2 + v_2^2 + v_3^2)$$

In general, $\langle \Psi_{sc} | \hat{N} | \Psi_{sc} \rangle = \sum_{k>0} 2 v_k^2$ population of $+k$ state

The expectation value of energy:

Fröhlich e-e attractive int.

$$\hat{H} = \underbrace{\sum_k \varepsilon_k \hat{a}_k^\dagger \hat{a}_k}_{\hat{O}_1} + \underbrace{\sum_{k>0} \sum_{\substack{k'>0 \\ k \neq k'}} V_{kk'} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k'} \hat{a}_{k'}}_{\hat{O}_2}$$

free electron

※ factor of 1/2 removed (cf. March) for $k>0$, $k'>0$ and counting $V_{1,2}$ and $V_{-1,-2}$ instead of $V_{1,2}$ and $V_{2,1}$

$$\langle \Psi_{sc} | \hat{O}_1 | \Psi_{sc} \rangle = 0 \cdot u_1^2 u_2^2 u_3^2 + 2\varepsilon_1 v_1^2 u_2^2 u_3^2 + \cdots + (2\varepsilon_1 + 2\varepsilon_2 + 2\varepsilon_3) v_1^2 v_2^2 v_3^2$$

$$= 2\varepsilon_1 v_1^2 + 2\varepsilon_2 v_2^2 + 2\varepsilon_3 v_3^2$$

In general, $\langle \Psi_{sc} | \hat{O}_1 | \Psi_{sc} \rangle = \sum_{k>0} 2 \varepsilon_k v_k^2$

$$\langle \Psi_{sc} | \hat{O}_2 | \Psi_{sc} \rangle_0 = \underset{\langle 000 | \hat{O}_2 | 000 \rangle}{0 \cdot u_1^2 u_2^2 u_3^2} + \underset{\langle 100 | \hat{O}_2 | 100 \rangle}{0 \cdot v_1^2 u_2^2 u_3^2} + \cdots = 0$$

zero-electron diff.

$\langle 100 | \hat{O}_2 | 100 \rangle$ etc.

$$\langle \Psi_{sc} | \hat{O}_2 | \Psi_{sc} \rangle_2 = \underset{\substack{\langle 100 | \hat{O}_2 | 010 \rangle \\ \langle 010 | \hat{O}_2 | 100 \rangle}}{(V_{12} + V_{-1,-2}) v_1 u_1 v_2 u_2 u_3^2} + \cdots + \underset{\substack{\langle 101 | \hat{O}_2 | 011 \rangle \\ \langle 011 | \hat{O}_2 | 101 \rangle}}{(V_{12} + V_{-1,-2}) v_1 u_1 v_2 u_2 v_3^2} + \cdots$$

two-electron diff.

$\langle 100 | \hat{O}_2 | 010 \rangle$ etc.

$$= 2V_{12} v_1 u_1 v_2 u_2 + 2V_{23} v_2 u_2 v_3 u_3 + 2V_{13} v_1 u_1 v_3 u_3$$

In general, $\langle \Psi_{sc} | \hat{O}_2 | \Psi_{sc} \rangle = \sum_{k>0} \sum_{\substack{k'>0 \\ k \neq k'}} V_{kk'} v_k u_k v_{k'} u_{k'}$

$$\langle \Psi_{sc} | \hat{H} | \Psi_{sc} \rangle = \sum_{k>0} 2 \varepsilon_k v_k^2 + \sum_{k>0} \sum_{\substack{k'>0 \\ k \neq k'}} V_{kk'} v_k u_k v_{k'} u_{k'}$$

1) Ground-state energy

We minimize $E = \langle \Psi_{sc} | \hat{H} | \Psi_{sc} \rangle = \sum_{k>0} 2 \epsilon_k v_k^2 + \sum_{k>0} \sum_{\substack{k'>0 \\ k \neq k'}} V_{kk'} v_k u_k v_{k'} u_{k'}$

w/ constraint $\langle \Psi_{sc} | \hat{N} | \Psi_{sc} \rangle = \sum_{k>0} 2 v_k^2 = \bar{N}$; $u_k^2 + v_k^2 = 1$

$$\mathcal{L} = E - \mu \left(\sum_{k>0} 2 v_k^2 - \bar{N} \right) = \sum_{k>0} 2 (\underbrace{\epsilon_k - \mu}_{\epsilon_k}) v_k^2 + \sum_{k>0} \sum_{\substack{k'>0 \\ k \neq k'}} V_{kk'} v_k u_k v_{k'} u_{k'} + \mu \bar{N}$$

chemical potential
Fermi energy

$\mu \to \epsilon_f$

w/ $v_k = \sin\theta_k$, $u_k = \cos\theta_k$

($\sin\theta_k = 1$ for $\epsilon_k \le \mu$, $= 0$ for $\epsilon_k > \mu$ is non SC state)

$$\mathcal{L} = \sum_{k>0} 2 \epsilon_k \sin^2\theta_k + \frac{1}{4} \sum_{k>0} \sum_{\substack{k'>0 \\ k \neq k'}} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} + \mu \bar{N}$$

At minimum,

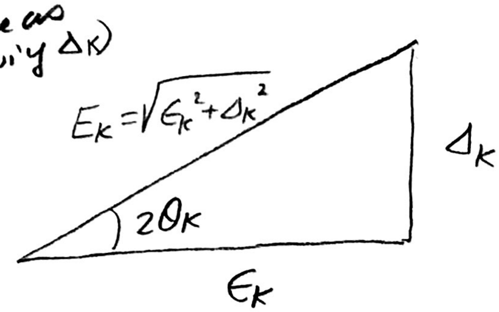
$$0 = \frac{\partial \mathcal{L}}{\partial \theta_k} = 2 \epsilon_k \sin 2\theta_k + \sum_{\substack{k'>0 \\ k' \neq k}} V_{kk'} \cos 2\theta_k \sin 2\theta_{k'}$$

Dividing w/ $2\epsilon_k \cos 2\theta_k$

$$\tan 2\theta_k = -\frac{1}{2\epsilon_k} \sum_{\substack{k'>0 \\ k' \neq k}} V_{kk'} \sin 2\theta_{k'} \quad \cdots ☆$$

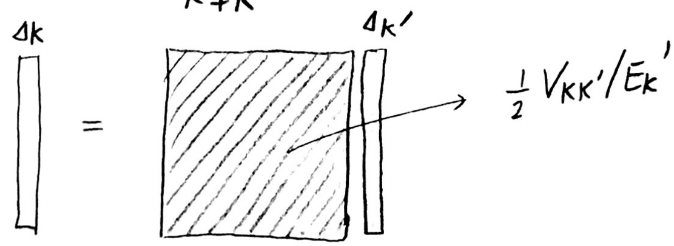
Setting $\tan 2\theta_k = \frac{\Delta_k}{\epsilon_k}$ (knowing θ_k is same as knowing Δ_k) $\longrightarrow$

$\sin 2\theta_k = \frac{\Delta_k}{E_k} \longleftarrow$



☆ becomes

$$\Delta_k = -\frac{1}{2} \sum_{\substack{k'>0 \\ k' \neq k}} V_{kk'} \frac{\Delta_{k'}}{E_{k'}} \quad \cdots\cdots ◎$$



Assuming

$$V_{kk'} = \begin{cases} -v & \mu-\delta < \varepsilon_k < \mu+\delta \\ & \text{(also } k>0, k'>0 \text{ or } k<0, k'<0 \text{ (cf. ⑤)} \\ & \text{and } k \neq k') \\ 0 & \end{cases}$$

⓪ becomes

$$\Delta_k = \frac{1}{2} \sum_{\substack{k'>0 \\ |\epsilon|<\delta}} v \frac{\Delta_{k'}}{E_{k'}} \longrightarrow$$

(constant of k)

same row repeated

$\Delta_1 = \Delta_2 = \cdots = \Delta_k$

Dividing w/ $\Delta_k = \Delta$

$$1 = \frac{v}{2} \sum_{\substack{k'>0 \\ |\epsilon|<\delta}} \frac{1}{E_{k'}}$$

(we solve this for Δ, which is in $E_{k'}$)
(later identified as 1/2 SC gap

$$\frac{2}{v} = \sum_{\substack{k'>0 \\ |\epsilon|<\delta}} \frac{1}{\sqrt{\epsilon^2+\Delta^2}}$$

density of states $\rho(\epsilon)$

constant in the thin shell

$$\text{Let } \sum_{\substack{k'>0 \\ |\epsilon|<\delta}} \rightarrow \int_{|\epsilon|<\delta} dk' \longrightarrow \int_{|\epsilon|<\delta} \frac{dk'}{d\epsilon} d\epsilon \longrightarrow \rho \int_{|\epsilon|<\delta} d\epsilon$$

momentum

cf. integrals table or Mathematica

$$⊗ \quad \frac{2}{v} = \rho \int_{-\delta}^{\delta} \frac{d\epsilon}{\sqrt{\epsilon^2+\Delta^2}} = \rho \left[\ln \left| \epsilon + \sqrt{\epsilon^2+\Delta^2} \right| \right]_{-\delta}^{\delta}$$

$$= \rho \ln \frac{\sqrt{\delta^2+\Delta^2}+\delta}{\sqrt{\delta^2+\Delta^2}-\delta}$$

$$e^{-2/\rho v} = \frac{\sqrt{\delta^2+\Delta^2}-\delta}{\sqrt{\delta^2+\Delta^2}+\delta}$$

$$e^{-2/\rho v}\left(\sqrt{\delta^2+\Delta^2}+\delta\right) = \sqrt{\delta^2+\Delta^2}-\delta$$

$$\delta\left(1+e^{-2/\rho v}\right) = \sqrt{\delta^2+\Delta^2}\left(1-e^{-2/\rho v}\right)$$

$$\frac{e^{1/\rho v}+e^{-1/\rho v}}{e^{1/\rho v}-e^{-1/\rho v}} = \frac{\sqrt{\delta^2+\Delta^2}}{\delta} \longrightarrow \frac{4+\left(e^{1/\rho v}-e^{-1/\rho v}\right)^2}{\left(e^{1/\rho v}-e^{-1/\rho v}\right)^2} = \frac{\delta^2+\Delta^2}{\delta^2}$$

$$\frac{2}{e^{1/\rho v}-e^{-1/\rho v}} = \frac{\Delta}{\delta} \longrightarrow \Delta = \delta \operatorname{csch} \frac{1}{\rho v}$$

when $e^{1/\rho v} \gg e^{-1/\rho v}$ $\quad \boxed{\Delta \approx 2\delta e^{-1/\rho v}}$

nonanalytic fxn of v
cannot be expanded
in a Taylor series!
No perturbation
theory

Now that we found θ_K minimizing E, we evaluate E

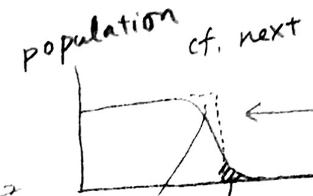
$$E_{sc} = \sum_{K>0} 2\,\varepsilon_K \sin^2\theta_K + \frac{1}{4}\sum_{K>0}\sum_{\substack{K'>0\\ K\neq K'}} V_{KK'} \sin 2\theta_K \sin 2\theta_{K'}$$

using ♣

$$= \sum_{K>0} 2\,\overset{\varepsilon_K-\mu}{\epsilon_K} \sin^2\theta_K - \frac{1}{2}\sum_{K>0} \epsilon_K \sin 2\theta_K \tan 2\theta_K + \mu\bar{N}$$

For non-SC state $\sin\theta_K = \begin{cases} 1 & \varepsilon_K \le \mu \text{ occ.} \\ 0 & \varepsilon_K > \mu \text{ vir.} \end{cases}$ either way $\begin{cases} \sin 2\theta_K = 0 \\ \tan 2\theta_K = 0 \end{cases}$

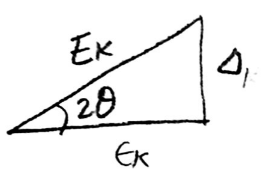
$$E_{non\text{-}sc} = \sum_{\substack{K>0\\ \varepsilon_K \le \mu}} 2\,\epsilon_K + \mu\bar{N}$$



cf. next page

So, the stabilization caused by Cooper pair formation is

$$E_{sc} - E_{non\text{-}sc} = \sum_{K>0} 2\,\epsilon_K \sin^2\theta_K - \frac{1}{2}\sum_{K>0} \epsilon_K \sin 2\theta_K \tan 2\theta_K - \sum_{\substack{K>0\\ \varepsilon_K\le\mu}} 2\,\epsilon_K$$



$$\underbrace{\sin^2\theta_K = \frac{1-\cos 2\theta_K}{2} = \frac{1}{2} - \frac{\epsilon_K}{2E_K},\quad \sin 2\theta_K = \frac{\Delta}{E_K},\quad \tan 2\theta_K = \frac{\Delta}{\epsilon_K}}_{|\epsilon_K|<\delta \ (\text{elsewhere } \sin^2\theta_K = 1 \text{ for } \varepsilon_K \le \mu)}$$

$$E_{sc} - E_{non\text{-}sc} = \sum_{-\delta<\epsilon_K<0}\left(-\epsilon_K - \frac{\epsilon_K}{E_K}\right) + \sum_{0<\epsilon_K<\delta}\left(\epsilon_K - \frac{\epsilon_K}{E_K}\right) - \sum_{K>0}\frac{\Delta^2}{2E_K}$$

$$= \rho\int_{-\delta}^{0} d\epsilon\left(-\epsilon - \frac{\epsilon^2}{\sqrt{\epsilon^2+\delta^2}}\right) + \rho\int_{0}^{\delta} d\epsilon\left(\epsilon - \frac{\epsilon^2}{\sqrt{\epsilon^2+\Delta^2}}\right) - \rho\int_{-\delta}^{\delta} d\epsilon\,\frac{\Delta^2}{2\sqrt{\epsilon^2+\Delta^2}}$$

$$= 2\rho\int_0^{\delta} d\epsilon\left(\epsilon - \frac{\epsilon^2}{\sqrt{\epsilon^2+\Delta^2}}\right) - \frac{\rho\Delta^2}{v}$$

use ♒

use Mathematica

$$= \rho\left[\epsilon^2 - \epsilon\sqrt{\epsilon^2+\Delta^2} + \Delta^2 \tanh^{-1}\frac{\epsilon}{\sqrt{\epsilon^2+\Delta^2}}\right]_0^{\delta} - \frac{\rho\Delta^2}{v}$$

cancels $\because \tanh^{-1}x = \frac{1}{2}\ln\frac{1+x}{1-x}$

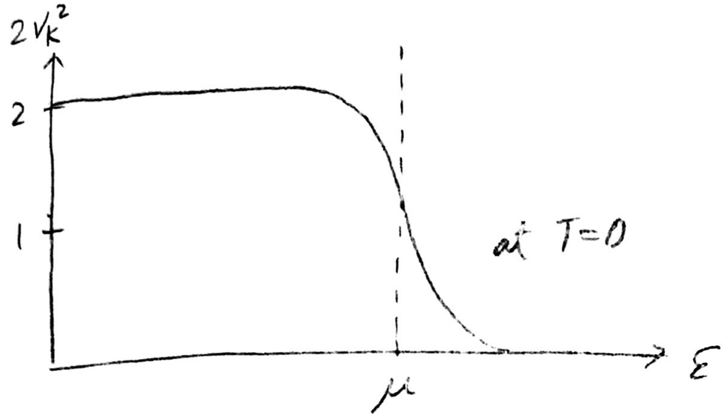
$$= \rho\left(\delta^2 - \delta\sqrt{\delta^2+\Delta^2}\right)$$

$$\approx \boxed{-\frac{\rho\Delta^2}{2}}$$ stabilization! (SC state more stable than non-SC)

2) Population

The occupation number of the k^{th} orbitals $\overline{k,\uparrow}$ $\overline{-k,\downarrow}$ is $2v_k^2$

$$2v_k^2 = 2\sin^2\theta_k = 1 - \frac{\epsilon_k}{E_k} = 1 - \frac{\varepsilon_k - \mu}{\sqrt{(\varepsilon_k-\mu)^2+\Delta^2}}$$



cf. Fermi-Dirac occupancy

$$\frac{2}{1+\exp\{(\varepsilon_k-\mu)/k_BT\}}$$

3) Excitation

If we define new operators (Bogoliubov transformation)

$$\hat{\alpha}_k^\dagger = u_k \hat{a}_k^\dagger - v_k \hat{a}_{-k}, \quad \hat{\alpha}_{-k}^\dagger = u_k \hat{a}_{-k}^\dagger + v_k \hat{a}_k$$

(*) derivation later

we can rewrite the free energy operator as

$$\hat{F} = \hat{H} - \mu\hat{N} = \sum_k \underbrace{\epsilon_k}_{\varepsilon_k-\mu} \hat{a}_k^\dagger \hat{a}_k + \sum_{k>0}\sum_{\substack{k'>0 \\ k\neq k'}} V_{kk'} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-k'} \hat{a}_{k'}$$

$$= \underbrace{E_{sc}}_{\text{superconducting g.s. energy}} - \mu\bar{N} + \sum_k \underbrace{E_k}_{\sqrt{\epsilon_k^2+\Delta^2}} \underbrace{\{\hat{\alpha}_k^\dagger \hat{\alpha}_k\}}_{\text{normal ordered}} + (\text{small terms})$$

energy band (energy vs. momentum)

compare

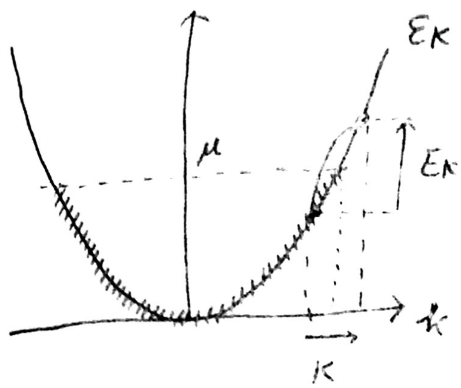
$$\hat{H} = E_{HF} + \sum_p \varepsilon_p \{\hat{p}^\dagger \hat{p}\} + \frac{1}{4}\sum_{p,q,r,s} \langle pq||rs\rangle \{\hat{p}^\dagger \hat{q}^\dagger \hat{s} \hat{r}\}$$

energy band (energy vs. momentum)

as we will show $\hat{\alpha}_k |\Psi_{sc}\rangle = 0$, so $\hat{\alpha}_k^\dagger |\Psi_{sc}\rangle$ is an excited state whose energy is

$$E_k \langle \Psi_{sc} | \{\hat{\alpha}_k\}\{\hat{\alpha}_k^\dagger \hat{\alpha}_k\}\{\hat{\alpha}_k^\dagger\} | \Psi_{sc}\rangle$$

Further, $\hat{\alpha}_k^\dagger = \underbrace{u_k \hat{a}_k^\dagger}_{\substack{\text{create} \\ k,\uparrow}} - \underbrace{v_k \hat{a}_k}_{\substack{\text{annihilate} \\ -k,\downarrow}} \rightarrow$ eitherway, momentum k spin $\uparrow$



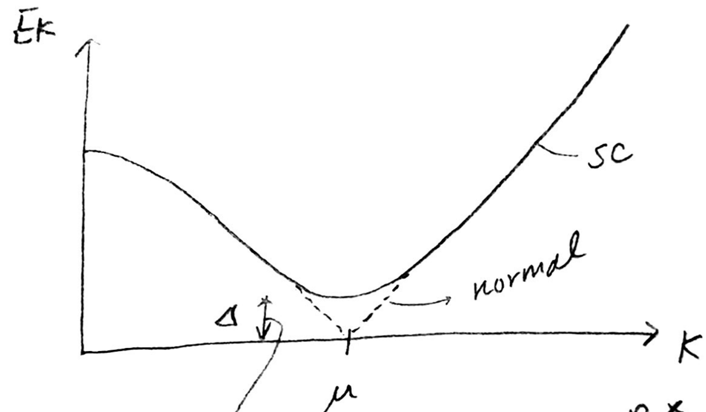
For normal metal, $\Delta = 0$

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2} = \sqrt{(\varepsilon_k - \mu)^2} = |\varepsilon_k - \mu|$$

For SC, $\Delta > 0$

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2} = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2} \sim \Delta \text{ at } \varepsilon_k = \mu$$

folding ε_k at μ



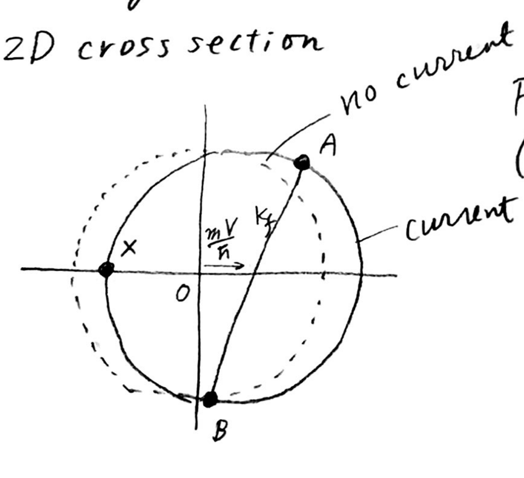
superconducting gap $\times$ ½

scattering of an electron by phonon/defect needs energy to break the cooper pair

$\Rightarrow$ no scattering or Ohmic resistence!

Looking from above

2D cross section



For Ohmic resistence to occur, scattering of Cooper pair $(A,B) \rightarrow (X,X)$ has to be energetically favorable,

Energy gain: $\frac{\hbar^2}{2m} OA^2 + \frac{\hbar^2}{2m} OB^2 - 2 \cdot \frac{\hbar^2}{2m} OX^2 = 2\hbar k_f V$

Energy loss: 2Δ (2 electrons excited from $\substack{A \to X \\ B \to X}$)

SC state: $V < \frac{\Delta}{\hbar k_f}$

Derivation of ※ (Bogoliubov transformation)

1) Confirm $\hat{\alpha}_k|\Psi_{sc}\rangle = 0$

Example) $|\Psi_{sc}\rangle = u_1u_2u_3|000\rangle + v_1u_2u_3|100\rangle + \cdots + v_1v_2v_3|111\rangle$

$$\hat{\alpha}_1|\Psi_{sc}\rangle = (u_1\hat{a}_1 - v_1\hat{a}_{-1}^\dagger)(u_1u_2u_3|000\rangle + v_1u_2u_3|100\rangle) + \cdots$$

$$= (u_1v_1u_2u_3 - v_1u_1u_2u_3) + \cdots$$

$k_1\uparrow$ $-k_1\downarrow$ $k_2\uparrow$ $-k_2\downarrow$ $k_3\uparrow$ $-k_3\downarrow$

$$= 0$$

2) Confirm $\hat{\alpha}_k^\dagger|\Psi_{sc}\rangle$ is normalized

Ex) $\hat{\alpha}_1^\dagger|\Psi_{sc}\rangle = (u_1\hat{a}_1^\dagger - v_1\hat{a}_{-1})(u_1u_2u_3|000\rangle + v_1u_2u_3|100\rangle) + \cdots$

$$= (u_1^2u_2u_3 + v_1^2u_2u_3) + \cdots$$

$k_1\uparrow$ $-k_1\downarrow$ $k_2\uparrow$ $-k_2\downarrow$ $k_3\uparrow$ $-k_3\downarrow$

$$= u_2u_3|\tfrac{1}{2}00\rangle + v_2u_3|\tfrac{1}{2}10\rangle + u_2v_3|\tfrac{1}{2}01\rangle + v_2v_3|\tfrac{1}{2}11\rangle$$

$$\langle\Psi_{sc}|\hat{\alpha}_1\hat{\alpha}_1^\dagger|\Psi_{sc}\rangle = u_2^2u_3^2 + v_2^2u_3^2 + u_2^2v_3^2 + v_2^2v_3^2 = (u_2^2+v_2^2)(u_3^2+v_3^2) = 1$$

3) Invert $\hat{a} \to \hat{\alpha}$ to $\hat{\alpha} \to \hat{a}$

$$\hat{a}_k = u_k\hat{\alpha}_k + v_k\hat{\alpha}_{-k}^\dagger, \quad \hat{a}_{-k}^\dagger = u_k\hat{\alpha}_{-k}^\dagger - v_k\hat{\alpha}_k$$

4) Define the normal order of $\{\hat{\alpha}\}$ to be that in which all $\hat{\alpha}_k$ appear to the right of $\hat{\alpha}_k^\dagger$, so that

$$N_\alpha[\underbrace{\hat{\alpha}_k^{(\dagger)}\cdots\hat{\alpha}_k^{(\dagger)}}_{\text{if there's at least one } \hat{\alpha}_k}]|\Psi_{sc}\rangle = 0$$

(cf. Lec. on normal order)

5) Transform $\hat{F}$ in normal order

$$\hat{F} = \hat{H} - \mu \hat{N} = \sum_{K} \epsilon_K \hat{a}_K^{\dagger} \hat{a}_K + \sum_{K>0} \sum_{\substack{K'>0 \\ K \neq K'}} V_{KK'} \hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}$$

normal order w.r.t $\hat{\alpha}$'s

5-1)
$$\hat{a}_K^{\dagger} \hat{a}_K = N_\alpha [\hat{a}_K^{\dagger} \hat{a}_K] + \hat{a}_K^{\dagger} \hat{a}_K$$

$$= N_\alpha \left[(u_K \hat{\alpha}_K^{\dagger} + v_K \hat{\alpha}_{-K})(u_K \hat{\alpha}_K + v_K \hat{\alpha}_{-K}^{\dagger}) \right]$$

$$+ \langle \Psi_{sc} | (u_K \hat{\alpha}_K^{\dagger} + v_K \hat{\alpha}_{-K})(u_K \hat{\alpha}_K + v_K \hat{\alpha}_{-K}^{\dagger}) | \Psi_{sc} \rangle$$

v_K^2, 0, 0

$$= u_K^2 \hat{\alpha}_K^{\dagger} \hat{\alpha}_K - v_K^2 \hat{\alpha}_{-K}^{\dagger} \hat{\alpha}_{-K} + u_K v_K \hat{\alpha}_K^{\dagger} \hat{\alpha}_{-K}^{\dagger} + u_K v_K \hat{\alpha}_{-K} \hat{\alpha}_K + v_K^2$$

5-2)
$$\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'} = N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}]$$

$$+ N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}] + N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}]$$

$$+ N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}]$$

Wick's theorem!

$\hat{a}^{\dagger}\hat{a}^{\dagger}$ not possible $\because \hat{a}^{\dagger} = \hat{\alpha}^{\dagger} + \hat{\alpha}$

$K \neq K'$ precludes $N_\alpha [\hat{a}_K^{\dagger} \hat{a}_K^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}]$ etc.

$$N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{K'} \hat{a}_{K'}] = \langle \Psi_{sc} | (u_K \hat{\alpha}_K^{\dagger} + v_K \hat{\alpha}_{-K})(u_K \hat{\alpha}_{-K}^{\dagger} - v_K \hat{\alpha}_K) | \Psi_{sc} \rangle \quad \text{— ⓐ}$$

$u_K v_K$, 0, 0

$$\times N_\alpha \left[(u_{K'} \hat{\alpha}_{-K'} - v_{K'} \hat{\alpha}_{K'}^{\dagger})(u_{K'} \hat{\alpha}_{K'} + v_{K'} \hat{\alpha}_{-K'}^{\dagger}) \right]$$

$$= u_K v_K \left(u_{K'}^2 \hat{\alpha}_{-K'} \hat{\alpha}_{K'} - v_{K'}^2 \hat{\alpha}_{K'}^{\dagger} \hat{\alpha}_{-K'}^{\dagger} - u_{K'} v_{K'} \hat{\alpha}_{K'}^{\dagger} \hat{\alpha}_{K'} - u_{K'} v_{K'} \hat{\alpha}_{-K'}^{\dagger} \hat{\alpha}_{-K'} \right)$$

$$N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{K'} \hat{a}_{K'}] = \langle \Psi_{sc} | (u_{K'} \hat{\alpha}_{-K'} - v_{K'} \hat{\alpha}_{K'}^{\dagger})(u_{K'} \hat{\alpha}_{K'} + v_{K'} \hat{\alpha}_{-K'}^{\dagger}) | \Psi_{sc} \rangle \quad \text{— ⓑ}$$

$u_{K'} v_{K'}$, 0, 0

$$\times N_\alpha \left[(u_K \hat{\alpha}_K^{\dagger} + v_K \hat{\alpha}_{-K})(u_K \hat{\alpha}_{-K}^{\dagger} - v_K \hat{\alpha}_K) \right]$$

$$= u_{K'} v_{K'} \left(u_K^2 \hat{\alpha}_K^{\dagger} \hat{\alpha}_{-K}^{\dagger} - v_K^2 \hat{\alpha}_{-K} \hat{\alpha}_K - u_K v_K \hat{\alpha}_K^{\dagger} \hat{\alpha}_K - u_K v_K \hat{\alpha}_{-K}^{\dagger} \hat{\alpha}_{-K} \right)$$

$$N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{K'} \hat{a}_{K'}] = ⓐ \times ⓑ = u_K v_K u_{K'} v_{K'}$$

For later use

$$N_\alpha [\hat{a}_K^{\dagger} \hat{a}_{-K}^{\dagger} \hat{a}_{-K'} \hat{a}_{K'}] = 4 u_K v_K u_{K'} v_{K'} \hat{\alpha}_K^{\dagger} \hat{\alpha}_{-K'}^{\dagger} \hat{\alpha}_{-K} \hat{\alpha}_K + (\hat{\alpha}^{\dagger}\hat{\alpha}^{\dagger}\hat{\alpha}^{\dagger}\hat{\alpha}^{\dagger},\ \hat{\alpha}\hat{\alpha}\hat{\alpha}\hat{\alpha},\ \hat{\alpha}^{\dagger}\hat{\alpha}\hat{\alpha}\hat{\alpha},\ \hat{\alpha}\hat{\alpha}\hat{\alpha}\hat{\alpha})$$

$\cdots$ ⑤

5-3)

$$\hat{F} = \underbrace{\sum_{k} \epsilon_k v_k^2 + \sum_{\substack{k>0 \\ k\neq k'}} \sum_{k'>0} V_{kk'} u_k v_k u_{k'} v_{k'}}_{\to E_{sc} - \mu \bar{N}}$$

$$+ \sum_{k} \epsilon_k (u_k^2 - v_k^2)\, \hat{\alpha}_k^\dagger \hat{\alpha}_k - 4 \sum_{\substack{k>0 \\ k\neq k'}} \sum_{k'>0} V_{kk'} u_k v_k u_{k'} v_{k'}\, \hat{\alpha}_k^\dagger \hat{\alpha}_k$$

$$+ \sum_{k} \epsilon_k u_k v_k \left(\hat{\alpha}_k^\dagger \hat{\alpha}_{-k}^\dagger + \hat{\alpha}_{-k} \hat{\alpha}_k\right) + \sum_{\substack{k>0 \\ k\neq k'}} \sum_{k'>0} V_{kk'} u_{k'} v_{k'} (u_k^2 - v_k^2) \left(\hat{\alpha}_k^\dagger \hat{\alpha}_{-k}^\dagger + \hat{\alpha}_{-k} \hat{\alpha}_k\right)$$

$$+ (\text{small terms})$$

$$= E_{sc} - \mu \bar{N} + \sum_{k>0} h_k^{11}\, \hat{\alpha}_k^\dagger \hat{\alpha}_k + \sum_{k>0} h_k^{20} \left(\hat{\alpha}_k^\dagger \hat{\alpha}_{-k}^\dagger + \hat{\alpha}_{-k} \hat{\alpha}_k\right) + (\text{small terms})$$

$$h_k^{11} = 2\epsilon_k (u_k^2 - v_k^2) - 4 \sum_{\substack{k'>0 \\ k'\neq k}} V_{kk'} u_k v_k u_{k'} v_{k'}$$

$$h_k^{20} = 2\epsilon_k u_k v_k + \sum_{\substack{k'>0 \\ k'\neq k}} V_{kk'} u_{k'} v_{k'} (u_k^2 - v_k^2)$$

$$= \epsilon_k \sin 2\theta_k + \sum_{\substack{k'>0 \\ k'\neq k}} V_{kk'} \frac{\sin 2\theta_{k'}}{2} \cos 2\theta_k = 0 \left(= \frac{\partial}{\partial \theta_k}(E_{sc} - \mu \bar{N})\right)$$

see above ⑥ 1)

Brillouin condition?

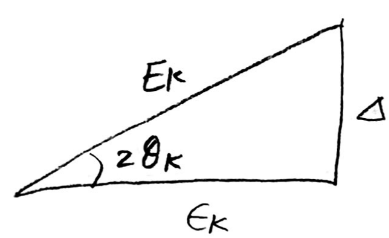
$$h_k^{11} = 2\epsilon_k \cos 2\theta_k - \sum_{\substack{k'>0 \\ k\neq k'}} V_{kk'} \sin 2\theta_{k'} \sin 2\theta_k$$

$$= 2\epsilon_k \cos 2\theta_k + 2\epsilon_k \tan 2\theta_k \sin 2\theta_k$$

used ✡ in ⑥ 1)

$$= \frac{2\epsilon_k^2}{E_k} + 2\epsilon_k \frac{\Delta}{\epsilon_k} \frac{\Delta}{E_k}$$

$$= \frac{2(\epsilon_k^2 + \Delta^2)}{E_k} = 2E_k$$



Hence, $\hat{F} = E_{sc} - \mu \bar{N} + \sum_{k>0} 2E_k\, \hat{\alpha}_k^\dagger \hat{\alpha}_k + (\text{small terms})$

$$= E_{sc} - \mu \bar{N} + \sum_{k} E_k \underbrace{\{\hat{\alpha}_k^\dagger \hat{\alpha}_k\}}_{\text{n.o. does nothing}} + (\text{small terms})$$

6) Elevated temperature BCS

$$\hat{F} = E_{SC} - \mu\bar{N} + \sum_{k>0} 2E_k \hat{\alpha}_k^{\dagger}\hat{\alpha}_k + 4\sum_{k>0}\sum_{\substack{k'>0\\ k\neq k'}} V_{kk'} u_k v_k u_{k'} v_{k'} \hat{\alpha}_k^{\dagger}\hat{\alpha}_{-k'}^{\dagger}\hat{\alpha}_{-k'}\hat{\alpha}_k$$

← from ⑤ ⑥ 5)

The free energy at T is (cf. finite-T HF theory)

$$F_{SC} = (E_{SC} - \mu\bar{N}) + \sum_{k>0} 2E_k f_k^- + 4\sum_{k>0}\sum_{\substack{k'>0\\ k\neq k'}} V_{kk'} u_k v_k u_{k'} v_{k'} f_k^- f_{k'}^-$$

$$- TS$$

↳ this will turn out to be Fermi-Dirac distribution fxn

$$f_k^- = \frac{1}{\exp(E_k/k_BT)+1}$$

This can be derived (see below)

$$\hookrightarrow -k_B \sum_k \{ f_k^- \ln f_k^- + (1-f_k^-)\ln(1-f_k^-) \}$$

This can also be derived ※

$$F_{HF} = E_{nuc} - \mu\bar{N} + \sum_p \varepsilon_p f_p^- - \frac{1}{2}\sum_p\sum_q \langle pq||pq\rangle f_p^- f_q^-$$

$$+ k_BT \sum_p \{ f_p^- \ln f_p^- + (1-f_p^-)\ln(1-f_p^-) \}$$

Minimize F_{SC} by first varying θ_k then f_k^-

$$F_{SC} = \sum_{k>0} \left(2\epsilon_k \sin^2\theta_k \right) + \frac{1}{4}\sum_{k>0}\sum_{\substack{k'>0\\ k\neq k'}} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} \qquad \leftarrow E_{SC} - \mu\bar{N}$$

ⓐ ⓑ

$$+ \sum_{k>0} \left\{ 2\epsilon_k \cos 2\theta_k - \sum_{k'} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} \right\} f_k^- \qquad \leftarrow 2E_k f_k^-$$

see last page

$$+ \sum_{k>0}\sum_{\substack{k'>0\\ k\neq k'}} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} f_k^- f_{k'}^- \qquad \leftarrow 4\Sigma\Sigma\, Vuvuvff$$

$$+ k_BT \sum_{k>0} 2\{ f_k^- \ln f_k^- + (1-f_k^-)\ln(1-f_k^-) \} \qquad \leftarrow -TS$$

(a) $2\epsilon_k \sin^2\theta_k + 2\epsilon_k \cos 2\theta_k f_k^-$

$$= \epsilon_k(1-\cos 2\theta_k) + \epsilon_k \cos 2\theta_k \, 2f_k^-$$

$$= \epsilon_k - \epsilon_k \cos 2\theta_k (1-2f_k^-)$$

(b) $\frac{1}{4}\sum_{k>0}\sum_{k'>0} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} - \sum_{k>0}\sum_{k'>0} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} f_k^-$

$$+ \sum_{k>0}\sum_{k'>0} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} f_k^- f_{k'}^-$$

$$= \frac{1}{4}\sum_{k>0}\sum_{k'>0} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} (1-2f_k^-)(1-2f_{k'}^-)$$

$$F_{sc} = \sum_{k>0} \epsilon_k - \sum_{k>0} \epsilon_k \cos 2\theta_k (1-2f_k^-)$$

$$+ \frac{1}{4}\sum_{k>0}\sum_{k'>0} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} (1-2f_k^-)(1-2f_{k'}^-)$$

$$+ k_B T \sum_{k>0} 2\{ f_k^- \ln f_k^- + (1-f_k^-)\ln(1-f_k^-)\}$$

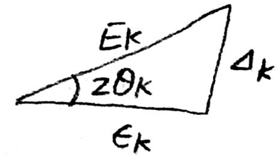
6-1) Varying θ_k $\quad \because \frac{\partial}{\partial \theta_k}$ can act on $\sin 2\theta_k$ and $\sin 2\theta_{k'}$

$$0 = \frac{\partial F_{sc}}{\partial \theta_k} = 2\epsilon_k \sin 2\theta_k (1-2f_k^-)$$

$$+ \sum_{k'>0} V_{kk'} \cos 2\theta_k \sin 2\theta_{k'} (1-2f_k^-)(1-2f_{k'}^-)$$

Dividing by $2\epsilon_k \cos 2\theta_k (1-2f_k^-)$

$$\tan 2\theta_k = -\frac{1}{2\epsilon_k}\sum_{k'>0} V_{kk'} \sin 2\theta_{k'} (1-2f_{k'}^-) \quad \text{— ✡}$$



$$\Delta_k = -\frac{1}{2}\sum_{k'>0} V_{kk'} \frac{\Delta_{k'}}{E_{k'}} (1-2f_{k'}^-)$$

6-2) Varying f_k^-

$$0 = \frac{\partial F_{sc}}{\partial f_k^-} = 2 \epsilon_k \cos 2\theta_k - \sum_{k'>0} V_{kk'} \sin 2\theta_k \sin 2\theta_{k'} (1 - 2 f_{k'}^-)$$

$$+ 2 k_B T \ln \frac{f_k^-}{1 - f_k^-}$$

Using ✡ 6-1)

$$-2 k_B T \ln \frac{f_k^-}{1-f_k^-} = 2 \epsilon_k \cos 2\theta_k + 2 \epsilon_k \sin 2\theta_k \tan 2\theta_k$$

$$= \frac{2 \epsilon_k}{\cos 2\theta_k} = 2 E_k$$

which we can solve for f_k^-

$$\frac{f_k^-}{1-f_k^-} = \exp(-E_k / k_B T)$$

$$f_k^- = \frac{1}{\exp(E_k / k_B T) + 1}$$

excitation energy
= excited-state energy
− μ

6-3) $$1 - 2 f_k^- = 1 - \frac{2}{\exp(E_k/k_B T) + 1} = \frac{\exp(E_k/k_BT) - 1}{\exp(E_k/k_BT) + 1} = \frac{\exp(E_k/2k_BT) - \exp(-E_k/2k_BT)}{\exp(E_k/2k_BT) + \exp(-E_k/2k_BT)}$$

$$= \tanh \frac{E_k}{2 k_B T}$$

Hence ✡ becomes

$$\Delta_k = -\frac{1}{2} \sum_{k'>0} V_{kk'} \frac{\Delta_{k'}}{E_{k'}} \tanh \frac{E_{k'}}{2 k_B T}$$

$\rightarrow 1 \quad (T \rightarrow 0)$

Same assumption $V_{KK'} = \begin{cases} -v & \mu-\delta < \varepsilon_K < \mu+\delta \\ 0 & \end{cases}$

Then $\Delta_K = \Delta$

$$\frac{2}{v} = \sum_{\substack{K'>0 \\ |\epsilon|<\delta}} \frac{1}{E_{K'}} \tanh \frac{E_{K'}}{2k_BT}$$

$$= \rho \int_{-\delta}^{\delta} \frac{d\epsilon}{\sqrt{\epsilon^2+\Delta^2}} \tanh \frac{\sqrt{\epsilon^2+\Delta^2}}{2k_BT} \quad \cdots\cdots \triangledown$$

As $T \to 0$, $\triangledown$ reverts to zero-temp. BCS eq. with SC gap ($\times\frac{1}{2}$) of $\Delta \approx 2\delta e^{-1/\rho V}$. When T is elevated, tanh $\ll 1$, and only root for Δ becomes $\Delta = 0$.
Let's call the smallest value of T which makes $\Delta = 0$ T_c. At $T = T_c$, $\triangledown$ is satisfied by $\Delta = 0$, hence

$$\frac{2}{\rho V} = \int_{-\delta}^{\delta} \frac{d\epsilon}{\epsilon} \tanh \frac{\epsilon}{2k_BT_c} \qquad x = \frac{\epsilon}{k_BT_c}$$

$$= 2\int_0^{\delta/k_BT_c} \frac{dx}{x} \tanh\frac{x}{2}$$

Exp[NIntegrate[$\frac{1}{X}$ Tanh[$\frac{X}{2}$],{X,0,100}]]
=113.387,
Exp[1000]
=1133.87

$$\exp(1/eV) \approx 1.13\,(\delta/k_BT)$$

$$k_BT_c \approx \underbrace{1.13\,\delta \exp(-1/\rho V)}_{\Delta/2} \approx \frac{2\Delta}{3.54} \leftarrow \text{SC gap at } T=0$$

※ Derivation of $S = -k_B \sum_i \{ f_i \ln f_i + (1-f_i) \ln (1-f_i) \}$

Entropy is defined as $S = k_B \ln W$, where W is the number of ways electrons fill the spinorbitals.

The i^{th} spinorbital is occupied by f_i electrons $(0 \le f_i \le 1)$.
To make the number of electrons an integer, we pretend that there are n_i states and $m_i = n_i f_i$ electrons,
↳ huge number

The number of ways to fill m_i electrons in n_i states is

$$ {}_{n_i}C_{m_i} = \frac{n_i!}{m_i!(n_i - m_i)!} $$

$$ S = k_B \ln W = k_B \ln \left(\prod_i \frac{n_i!}{m_i!(n_i-m_i)!} \right) $$

$$ = k_B \sum_i \left(\ln n_i! - \ln m_i! - \ln (n_i - m_i)! \right) $$

Using Striling's formula $\ln n_i! = n_i \ln n_i$

$$ = k_B \sum_i \left(n_i \ln n_i - m_i \ln m_i - (n_i - m_i) \ln (n_i - m_i) \right) $$

Setting $n_i = 1$, $m_i = n_i f_i = f_i$

$$ = -k_B \sum_i \left(f_i \ln f_i + (1-f_i) \ln (1-f_i) \right) $$