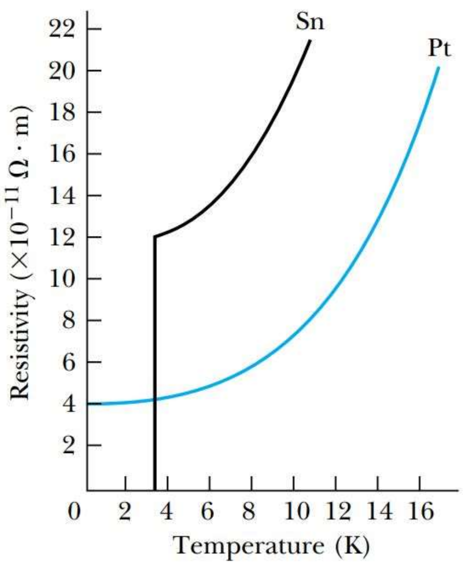
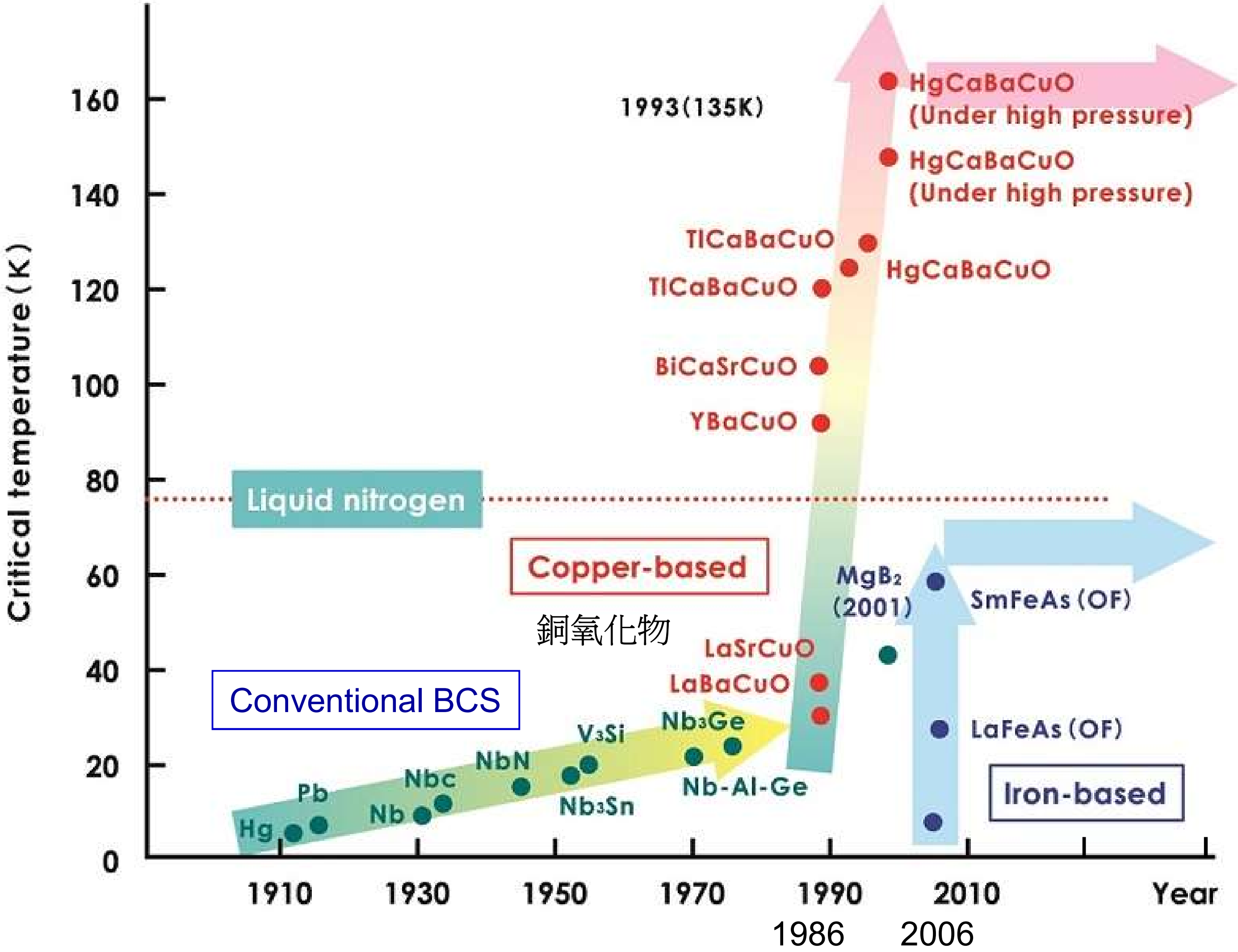


Superconducting transition temperatures and critical fields

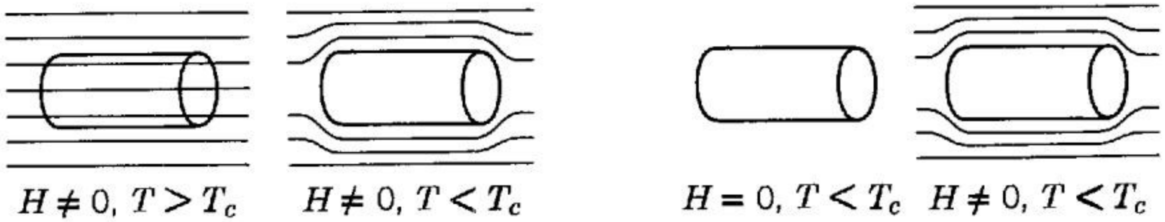
Upper number: Transition temperature in K
Lower number: Critical magnetic field at absolute zero in 10^{-4} tesla

Li	Be											B	C	N	O	F	Ne
Na	Mg											Al 1.18 105	Si	P	S	Cl	Ar
K	Ca	Sc	Ti 0.40 56	V 5.40 1408	Cr	Mn	Fe	Co	Ni	Cu	Zn 0.85 54	Ga 1.08 58	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr 0.61 47	Nb 9.25 2060	Mo 0.92 96	Tc 7.77 1410	Ru 0.49 69	Rh	Pd	Ag	Cd 0.52 28	In 3.41 282	Sn 3.72 505	Sb	Te	I	Xe
Cs	Ba	La 6.00 1046	Hf 0.13 13	Ta 4.47 829	W 0.02 1.15	Re 1.70 200	Os 0.66 70	Ir 0.11 16	Pt	Au	Hg 4.15 411	Tl 2.38 178	Pb 7.20 803	Bi	Po	At	Rn
Fr	Ra	Ac															

Families of superconductors

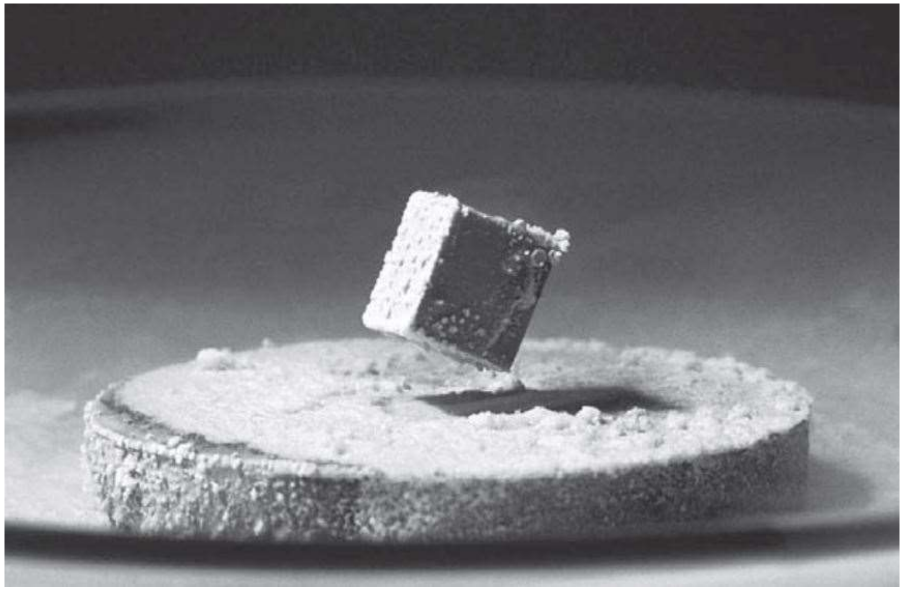


Meissner effect (Meissner and Ochsenfeld, 1933)



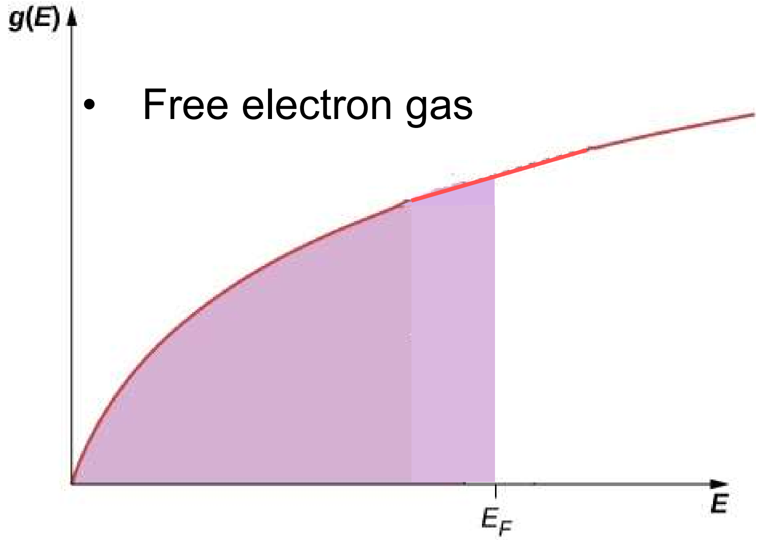
A superconductor is not just a perfect conductor, it's also a perfect diamagnet. This must be tested after measuring the resistance.

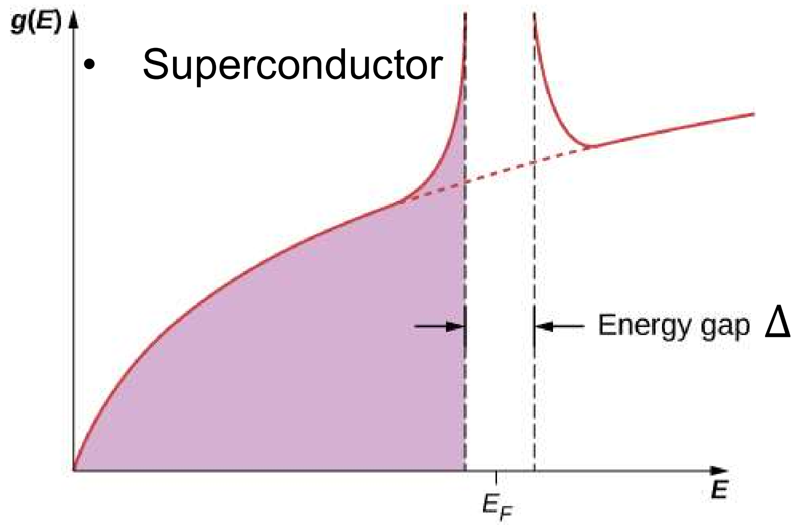
- Magnetic levitation



Superconducting energy gap

Density of states



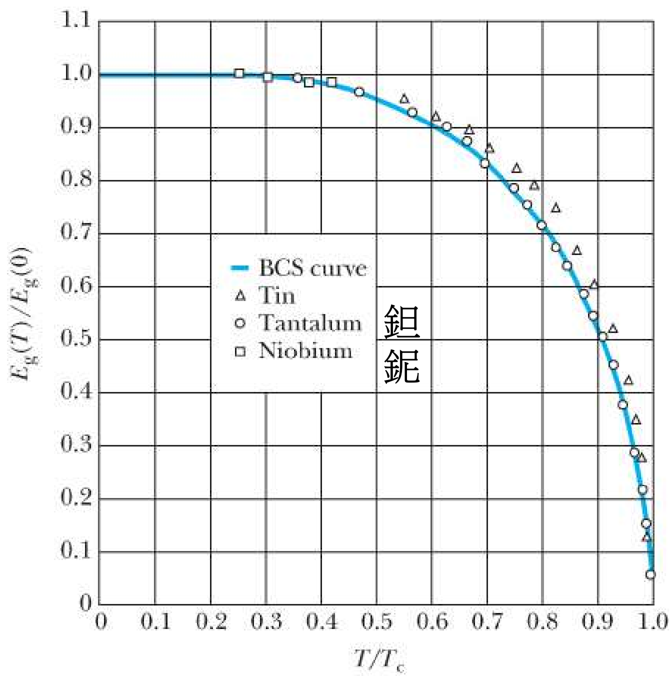


$$\Delta(0) \simeq 3.5\ kT_c$$

If $T_c = 4.2\ K$, then $\Delta(0) \simeq 10^{-3}\ eV$

- Universal behavior of $\Delta(T)$

$$\frac{\Delta(T)}{\Delta(0)} = 1.74\left(1 - \frac{T}{T_C}\right)^{1/2} \quad \text{for } T \approx T_C$$



- Connection between energy gap and T_c

  Δ's scale with different T_c's: $2\Delta(0) \sim 3.5\, k_B T_c$

MEASURED VALUES[a] OF $2\Delta(0)/k_B T_c$

ELEMENT	$2\Delta(0)/k_B T_c$
Al	3.4
Cd	3.2
Hg (α)	4.6
In	3.6
Nb	3.8
Pb	4.3
Sn	3.5
Ta	3.6
Tl	3.6
V	3.4
Zn	3.2

[a] $\Delta(0)$ is taken from tunneling experiments. Note that the BCS value for this ratio is 3.53. Most of the values listed have an uncertainty of ± 0.1.

What's the origin of superconductivity?

- A metal can (cannot) superconduct because its atoms can (cannot) superconduct?
  Neither Au nor Bi is superconductor, but alloy Au_2Bi is!
  White tin can, grey tin cannot! (the only difference is lattice structure)

- Good normal conductors (Cu, Ag, Au) are bad superconductor;
  bad normal conductors are good superconductors, why?
  What causes the superconducting gap?
- Failed attempts by many physicists: Bohr, Heisenberg, Born, Feynman …

A crucial hint:

- **Isotope effect** (1950):

It is found that $T_c = \text{const} \times M^{-\alpha}$

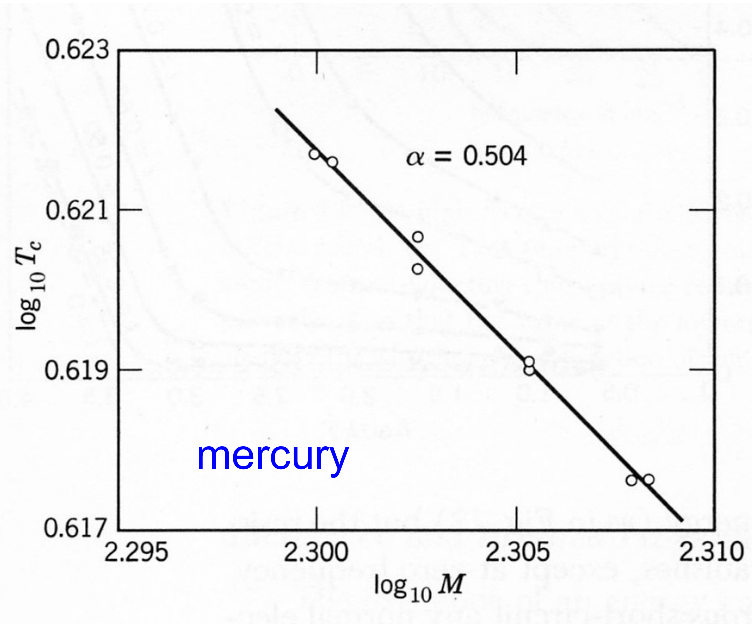
$\alpha \sim 1/2$ for different materials

$\leftrightarrow$ lattice vibration (?)

➡ **BCS theory**

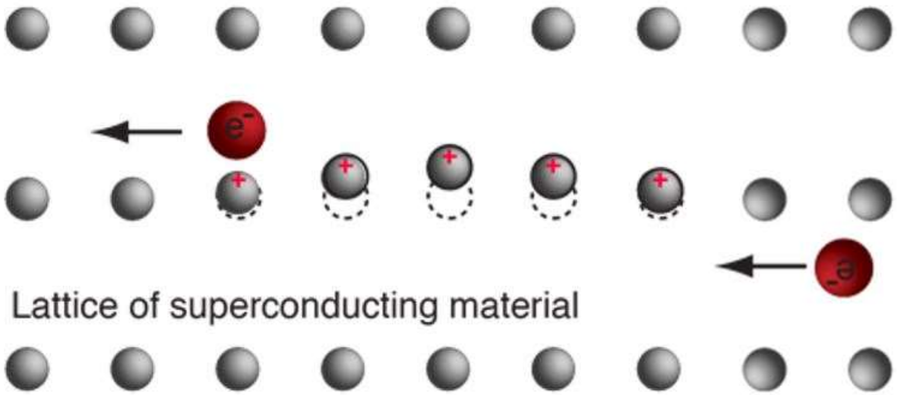
(Bardeen, Cooper, and Schrieffer 1957)

Bardeen Nobel 1956, 1972

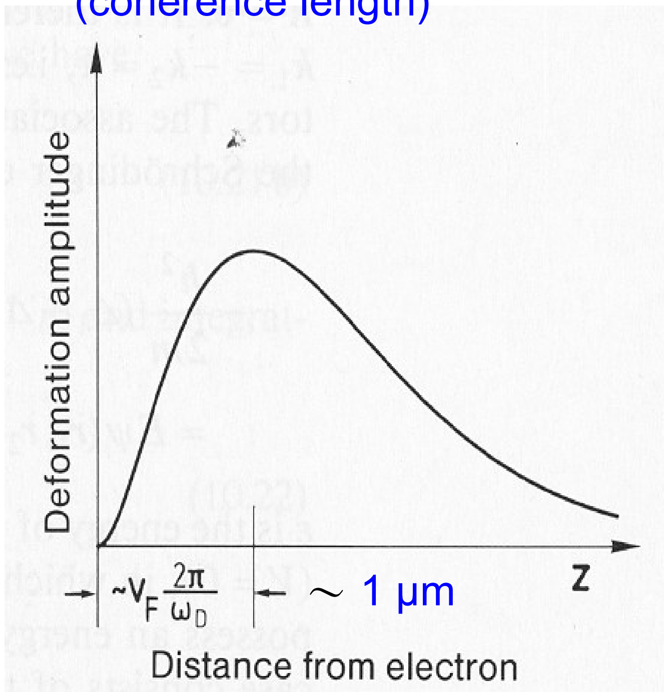


A crucial ingredient of BCS theory: **Cooper pair**

Dynamic electron-lattice interaction



Range of a Cooper pair (coherence length)



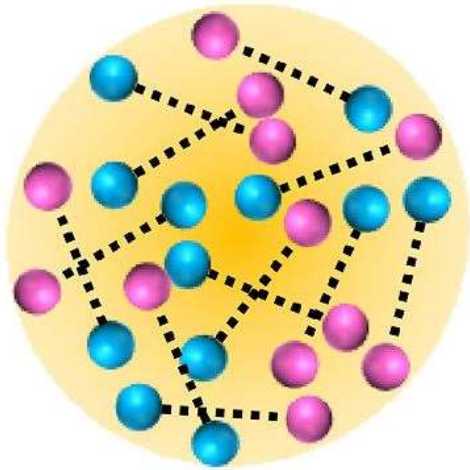
➡ Effective attractive interaction between 2 electrons (aka overscreening)

→ a Cooper pair of 2 electrons with opposite momenta (p↑,-p↓) (App. H of Kittel)

It takes 2Δ to break a Cooper pair

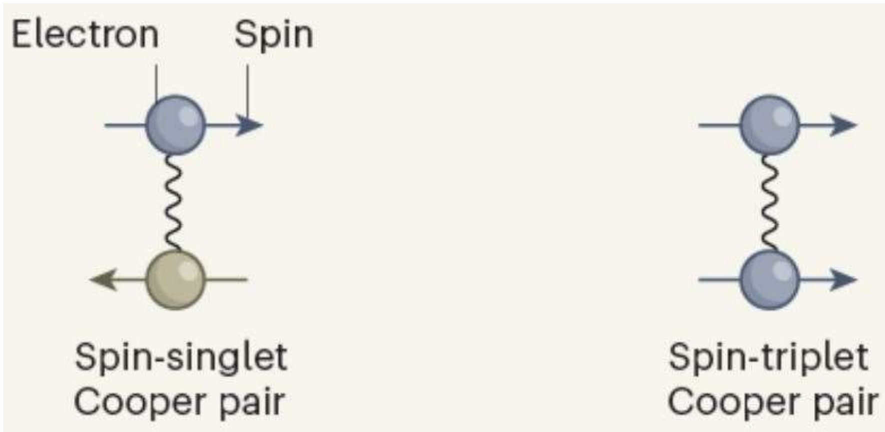
- These pairs are highly correlated and form a macroscopic condensate

- Fraction of electrons involved $\sim kT_c/E_F \sim 10^{-4}$
    - Average spacing between condensate electrons $\sim$ 10 nm
- Therefore, within the diameter of a Cooper pair, there are about $(1\mu m/10\ nm)^3 \sim 10^6$ other pairs. They form a very complex (but ordered) web.



- Symmetry of pairing

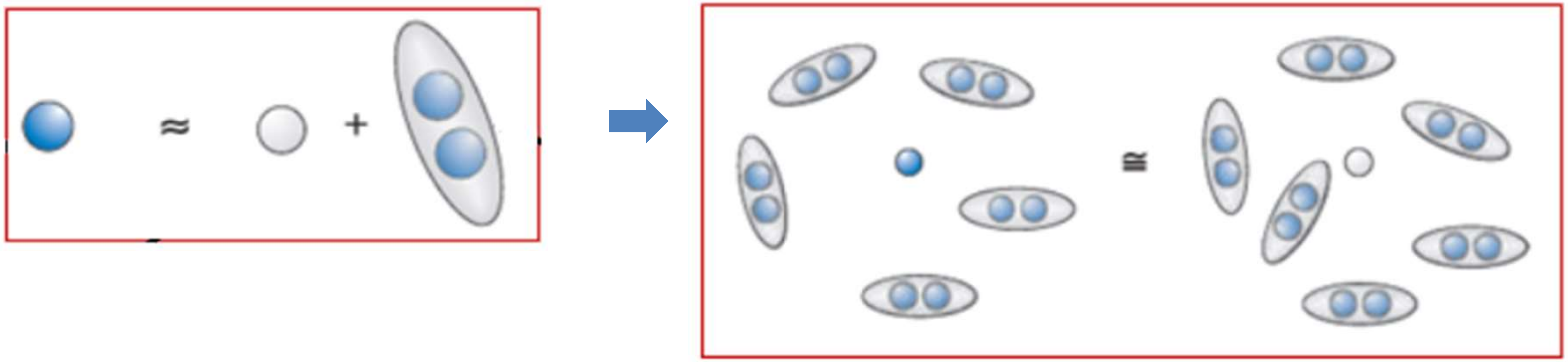
  Originally, Cooper used s-wave pairing, but other types of pairing are possible.



s-wave pairing   p-wave pairing

Particle-hole symmetry of superconductor

- A superconductor can be described with a macroscopic wave function with a definite phase ϕ. Because the number of particles N and the phase ϕ are conjugate variables (details later), the number of Cooper pairs are fluctuating.



Adding an electron is no different from adding a hole

In most of our discussions, a SC would be just like a narrow-gap semiconductor with particle-hole symmetry

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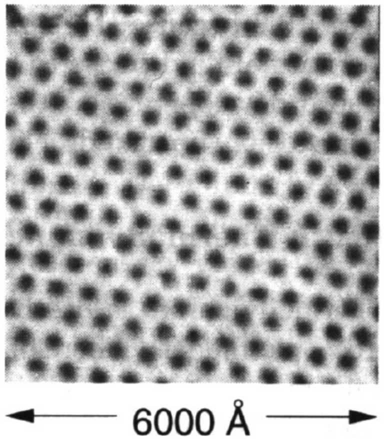
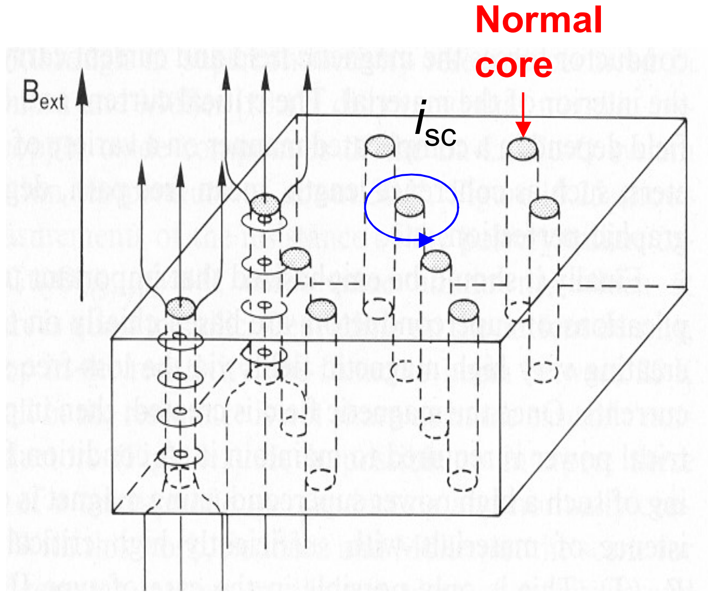
Type II SC (1935) – Nb, V, Tc, and alloys

Superconductor with vortex state

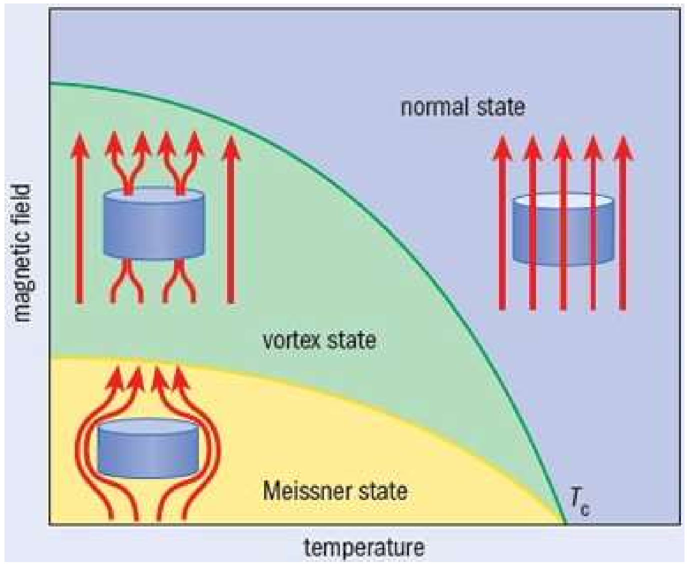


STM image $NbSe_2$, 1T, 1.8K



• The magnetic flux in a vortex is always quantized (flux quantum $\phi_0 = h/2e$)

• Large critical magnetic field. It remains superconducting up to 10~100 Tesla.



Review of BCS theory

A. Mean field Hamiltonian

   1. Bogoliubov transformation

B. BCS ground state

   1. Boson coherent state

   2. BCS coherent state

C. Excited states

D. Particle-hole symmetry

E. Real space formulation

Refs:

1. de Gennes, Superconductivity Of Metals And Alloys

2. Tinkham, Introduction to Superconductivity

First, basics of creation operators and annihilation operators

- Simple harmonic oscillator

$$a|n\rangle = \sqrt{n}|n-1\rangle$$
$$a^+|n\rangle = \sqrt{n+1}|n\rangle$$

- Fields as a collection of field quanta created by

$$\{a_{k_1}^+, a_{k_2}^+, a_{k_3}^+, \ldots\}$$

e.g, $$|\psi\rangle = a_{k_2}^+ \left(a_{k_5}^+\right)^2 \ldots |\mathbf{0}\rangle$$

$$[a_k, a_{k'}^+] = \delta_{kk'}$$ … etc for bosons

However, fermion operators use anticommutators

$$\{a_k, a_{k'}^+\} = \delta_{kk'}$$
$$\{a_k, a_{k'}\} = 0$$
$$\{a_k^+, a_{k'}^+\} = 0 \quad \rightarrow a_k^+ a_{k'}^+ = -a_{k'}^+ a_k^+$$
$$(a_k^+)^2 = 0$$

- Exchange 2 fermions flip the sign of the state
- Pauli exclusion principle

A. Mean field Hamiltonian

BCS Hamiltonian focuses on Cooper-pair electrons,

$$H_{MF} = \sum_{\mathbf{k}s} \varepsilon_k c^\dagger_{\mathbf{k}s} c_{\mathbf{k}s} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + \sum_{\mathbf{k}} \Delta^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$

$$\varepsilon_k = \hbar^2 k^2/2m - \mu$$

For the simplest type of s-wave SC, $\Delta_k = \Delta_0$.

Rewrite the first term,

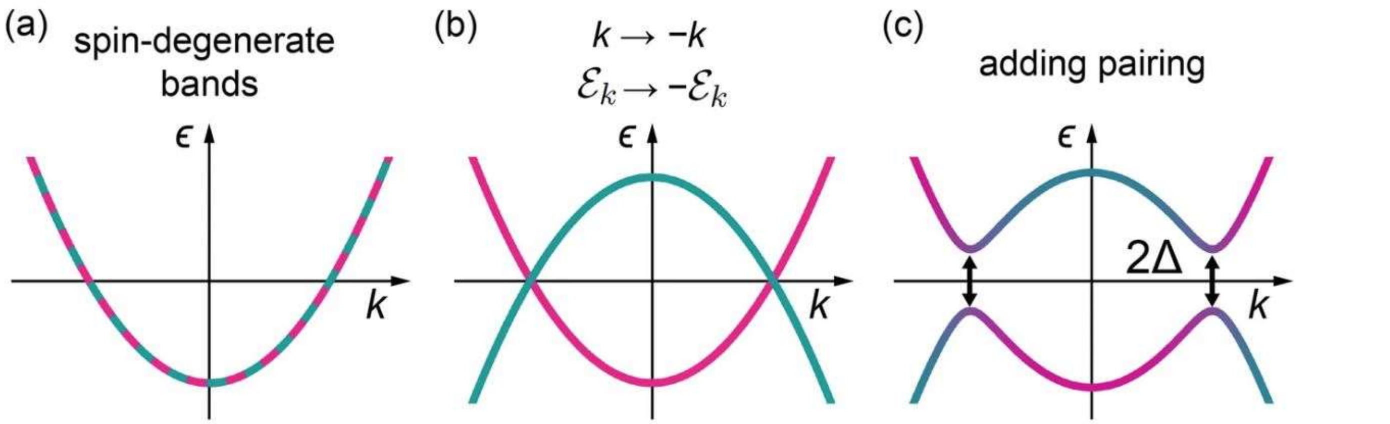
$$\sum_k \varepsilon_k \left(c^\dagger_{k\uparrow} c_{k\uparrow} - c_{k\downarrow} c^\dagger_{k\downarrow} \right) + \sum_k \varepsilon_k$$

$$\{c_{ks}, c^\dagger_{k's'}\} = \delta_{kk'}\delta_{ss'}, \quad \{c_{ks}, c_{k's'}\} = 0,$$

$$H_{MF} = \sum_k (c^\dagger_{k\uparrow} c_{-k\downarrow}) \begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta^*_k & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} + \sum_k \varepsilon_k$$

- Diagonalization of the Hamiltonian $$\begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta^*_k & -\varepsilon_k \end{pmatrix} = U \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} U^\dagger$$

Eigenvalues $$\pm E_k = \pm\sqrt{\varepsilon_k^2 + |\Delta_k|^2}$$



(keep only the positive excitation energy $+E_k$)

Figs from M. Hayes' article

Unitary matrix

$$U = \begin{pmatrix} \alpha_+ & \alpha_- \\ \beta_+ & \beta_- \end{pmatrix}$$

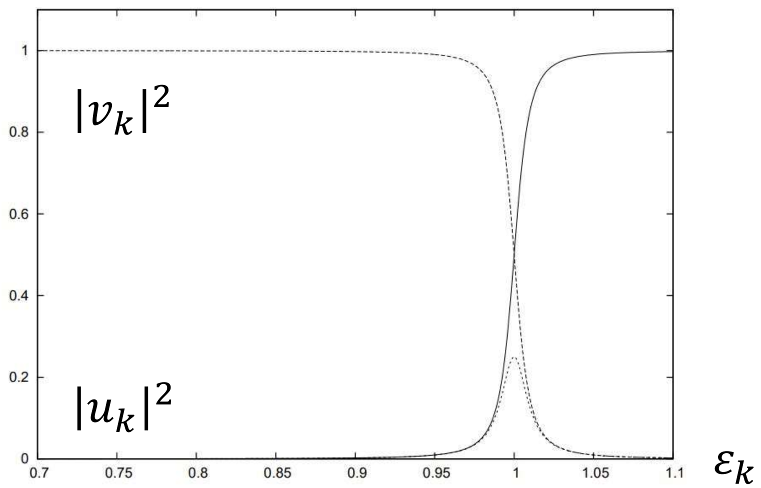
$$\alpha_+ = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right)}; \quad \beta_+ = -\sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)}\frac{\Delta_k^*}{|\Delta_k|}.$$

$$\alpha_- = \sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)}; \quad \beta_- = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right)}\frac{\Delta_k^*}{|\Delta_k|}.$$

Eigenvectors

$$\begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = \begin{pmatrix} u_k \\ v_k \end{pmatrix}, |u_k|^2 + |v_k|^2 = 1$$

$$\begin{pmatrix} \alpha_- \\ \beta_- \end{pmatrix} = \begin{pmatrix} -v_k^* \\ u_k \end{pmatrix}$$



Diagonalization with **Bogoliubov-Valatin transformation**

(a canonical transformation)

$$\begin{pmatrix} \gamma_{k1} \\ \gamma^{\dagger}_{-k2} \end{pmatrix} = U^{\dagger} \begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \end{pmatrix}$$

⟺

$$\begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \end{pmatrix} = U \begin{pmatrix} \gamma_{k1} \\ \gamma^{\dagger}_{-k2} \end{pmatrix} = \begin{pmatrix} u_k & -v_k^* \\ v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_{k1} \\ \gamma^{\dagger}_{-k2} \end{pmatrix}$$

With the requirement,
$$\{\gamma_{ks}, \gamma^{\dagger}_{k's'}\} = \delta_{kk'}\delta_{ss'},$$
$$\{\gamma_{ks}, \gamma_{k's'}\} = 0.$$

⇒

$$\begin{aligned} & H_{MF} \\ = & \sum_k (\gamma^{\dagger}_{k1} \gamma_{-k2}) \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \gamma_{k1} \\ \gamma^{\dagger}_{-k2} \end{pmatrix} + \sum_k \varepsilon_k \\ = & \sum_k E_k \left(\gamma^{\dagger}_{k1} \gamma_{k1} + \gamma^{\dagger}_{-k2} \gamma_{-k2} \right) + \text{const.} \end{aligned}$$

These QPs are not interacting

⇒ $$f(E_k) = \frac{1}{e^{E_k/kT} + 1}$$ Fermi-Dirac distribution

B. BCS ground state as a coherent state of Cooper pairs

First, 1. Boson coherent state

Recall a problem in Sakurai's Quantum Mechanics

Coherent state
$$|\lambda\rangle = e^{-|\lambda|^2/2} e^{\lambda a^\dagger}|0\rangle = e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}|n\rangle$$

Same as an oscillating Gaussian wavepacket

➡ $$a|\lambda\rangle = \lambda|\lambda\rangle, \quad \text{and} \quad \bar{n} = \langle\lambda|\hat{n}|\lambda\rangle = |\lambda|^2.$$

$$\lambda = |\lambda|e^{i\theta} = \sqrt{\bar{n}}e^{i\theta}$$

➡ $$\frac{1}{i}\frac{\partial}{\partial\theta}|\lambda\rangle = \hat{n}|\lambda\rangle$$

Therefore $\hat{n} \simeq \frac{1}{i}\frac{\partial}{\partial\theta}$ ➡ $\Delta n \Delta\theta \geq \frac{1}{2}$

Like *x* and *p*, *n* and θ are conjugate variables.

2. BCS coherent state

$$b_k^\dagger = c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$$ creates a Cooper pair

$$[A, BC] = \{A, B\}C - B\{A, C\}$$

➡ $$[b_k, b_{k'}^\dagger] = (1 - \hat{n}_{k\uparrow} - \hat{n}_{-k\downarrow})\,\delta_{kk'}$$ (Not exactly bosons)

$$\left(b_k^\dagger\right)^2 = 0$$ (Fermion character persists)

$$\begin{aligned} |\Psi_{BCS}\rangle &= e^{\sum_k \alpha_k b_k^\dagger}|0\rangle \\ &= \prod_k e^{\alpha_k b_k^\dagger}|0\rangle \\ &= \prod_k \left(1 + \alpha_k b_k^\dagger\right)|0\rangle \end{aligned}$$

After normalization, $$|\Psi_{BCS}\rangle = \prod_k \left(\tilde{u}_k + \tilde{v}_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger\right)|\mathbf{0}\rangle \qquad |\tilde{u}_k|^2 + |\tilde{v}_k|^2 = 1$$

Choose $\tilde{u}_k$ to be real, and $\tilde{v}_k$ can be complex

C. Excited states

- First, note that

$$\gamma_{k1}|\Psi_G\rangle = \left(u_k c_{k\uparrow} + v_k^* c_{-k\downarrow}^\dagger\right) \prod_{k'} \left(\tilde{u}_{k'} + \tilde{v}_{k'} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger\right) |\mathbf{0}\rangle$$

$$= 0 \quad \text{if } (\tilde{u}_k, \tilde{v}_k) = (u_k, -v_k^*).$$

BCS ground state can be seen as the state annihilated by the Bogoliubov operators:

$$\gamma_{k1}|\Psi_G\rangle = \gamma_{-k2}|\Psi_G\rangle = 0.$$

- Excited states (creation of Bogoliubov QPs)

$$\gamma_{k1}^\dagger|\Psi_G\rangle = c_{k\uparrow}^\dagger \prod_{k'\neq k} \left(u_{k'} - v_{k'}^* c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger\right) |\mathbf{0}\rangle,$$

$$\gamma_{-k2}^\dagger|\Psi_G\rangle = c_{-k\downarrow}^\dagger \prod_{k'\neq k} \left(u_{k'} - v_{k'}^* c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger\right) |\mathbf{0}\rangle.$$

For $\gamma_{k1}^\dagger$, it adds an electron to one of the states of $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$, which raises the energy (for the lack of Cooper binding energy). Similarly for the other operator $\gamma_{-k2}^\dagger$.

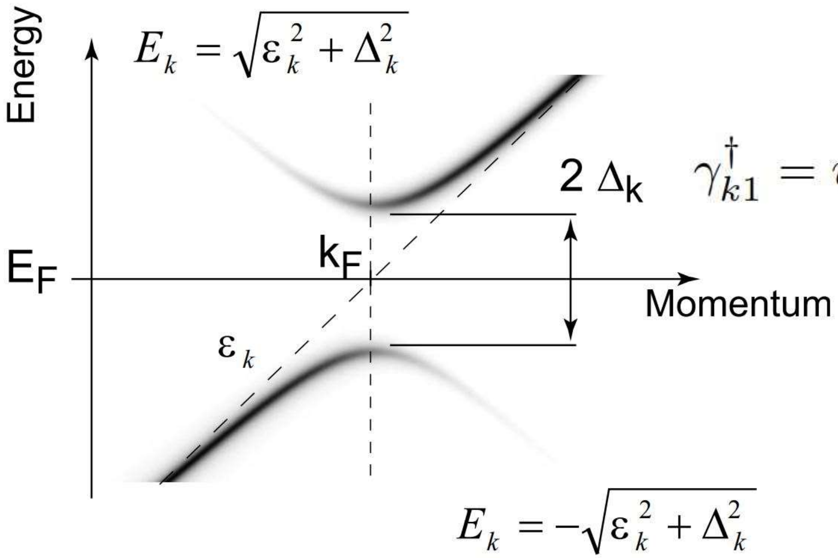
- Electron occupation

$$\langle \Psi_G | \sum_s c_{ks}^\dagger c_{ks} | \Psi_G \rangle = 2|v_k|^2$$

$$= 2 \to 0 \text{ as energy increases.}$$

$$\langle \Psi_G | \gamma_{k1} \sum_{s'} c_{ks'}^\dagger c_{ks'} \gamma_{k1}^\dagger | \Psi_G \rangle = 1$$

Compared to the ground state, the 1-bogolon state has one less electron below the Fermi energy, but one more electron above the Fermi energy. Therefore, the excited state moves one electron from below the Fermi energy to above.



$$\gamma_{k1}^\dagger = u_k c_{k\uparrow}^\dagger + v_k c_{-k\downarrow}$$

Fig from Balatsky et al, PRB 2009

D. Particle-hole symmetry

$$P(\mathbf{p}+e\mathbf{A})P^{-1} = -(\mathbf{p}-e\mathbf{A})$$

➡ $PiP^{-1} = -i$ PH operator P is an anti-unitary operator

if $\Delta_{-k} = \Delta_k$, then one has
(s-wave)

$$u_{-k} = u_k, \; v_{-k} = v_k.$$

if $\Delta_{-k} = -\Delta_k$, then
(p-wave)

$$u_{-k} = u_k, \; v_{-k} = -v_k.$$

For a s-wave SC, $\Delta_{-k} = \Delta_k$

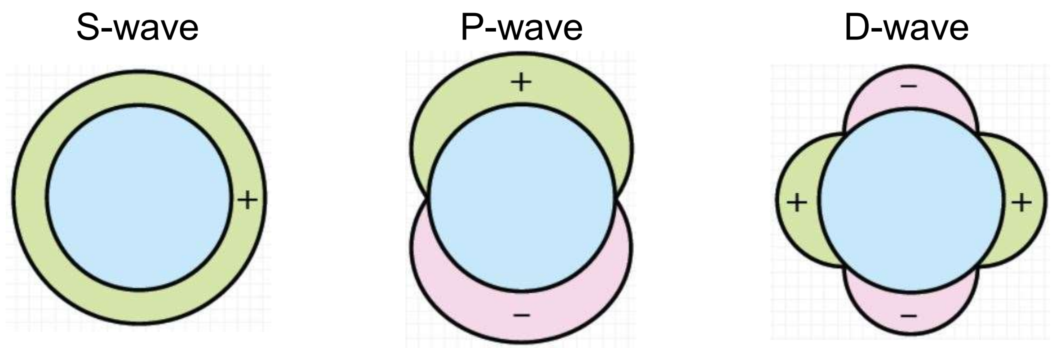
if $\psi_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$ has energy E_k,

then $P\psi_k = \begin{pmatrix} -v_k^* \\ u_k \end{pmatrix} = \begin{pmatrix} -v_{-k}^* \\ u_{-k} \end{pmatrix}$ has energy $-E_{-k}$.

we choose

$$P = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K = -i\tau_y K$$ ➡ $P^2 = -1$ For s-wave SC

Symmetry of gap function



Orbital angular momentum of Cooper pairs: 0, 1, 2

Figs from N. Curro's ppt

For a spinless p-wave SC, $\Delta_{-k} = -\Delta_k$

Simply the notation
$(c_{k\uparrow}, c^{\dagger}_{-k\downarrow}) \rightarrow (c_k, c^{\dagger}_{-k})$

if $\psi_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$ has energy E_k,

then $P\psi_k = \begin{pmatrix} v_k^* \\ u_k \end{pmatrix} = \begin{pmatrix} -v^*_{-k} \\ u_{-k} \end{pmatrix}$ has energy $-E_{-k}$.

we choose

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K = \tau_x K \quad \Rightarrow \quad P^2 = 1$$

For p-wave SC

If a system has particle-hole symmetry, then

$$P\mathsf{H}(\mathbf{k})P^{-1} = -\mathsf{H}(-\mathbf{k}).$$

To deal with vortices, edges … etc, we need

E. Real space formulation (Chap 5 of de Gennes)

$$\begin{aligned}\{\psi_s(\mathbf{r}), \psi_{s'}(\mathbf{r}')^\dagger\} &= \delta(\mathbf{r}-\mathbf{r}')\delta_{ss'}, \\ \{\psi_s(\mathbf{r}), \psi_{s'}(\mathbf{r}')\} &= 0.\end{aligned}$$

For s-wave,

(follow de Gennes's choice of the sign of Δ)

$$H_{eff} = \int d^3r \left\{ \sum_{s=\uparrow,\downarrow} \psi_s^\dagger H_0 \psi_s + \Delta(\mathbf{r})\psi_\uparrow^\dagger \psi_\downarrow^\dagger + \Delta^*(\mathbf{r})\psi_\downarrow\psi_\uparrow \right\}$$

$$H_0 = \frac{1}{2m}(\mathbf{p}+e\mathbf{A})^2 + V(\mathbf{r}) - \mu$$

Bogoliubov-Valatin transformation,

$$\begin{aligned}\psi_\uparrow(\mathbf{r}) &= \sum_{n\geq 0}\left(u_n(\mathbf{r})\gamma_{n\uparrow} - v_n^*(\mathbf{r})\gamma_{n\downarrow}^\dagger\right), \\ \psi_\downarrow^\dagger(\mathbf{r}) &= \sum_{n\geq 0}\left(v_n(\mathbf{r})\gamma_{n\uparrow} + u_n^*(\mathbf{r})\gamma_{n\downarrow}^\dagger\right).\end{aligned}$$

$$\Rightarrow \quad H_{eff} = \sum_{n,s} E_n \gamma_{ns}^\dagger \gamma_{ns}$$

demand that

$$\begin{aligned} \{\gamma_{ns}, \gamma^\dagger_{n's'}\} &= \delta_{nn'}\delta_{ss'}, \\ \{\gamma_{ns}, \gamma_{n's'}\} &= 0. \end{aligned}$$

$$\Rightarrow \begin{cases} i\hbar\dot{\gamma}_{ns} = [\gamma_{ns}, H_{eff}] = E_n\gamma_{ns}, \\ i\hbar\dot{\gamma}^\dagger_{ns} = \left[\gamma^\dagger_{ns}, H_{eff}\right] = -E_n\gamma^\dagger_{ns}. \end{cases}$$

On the other hand, $\begin{cases} i\hbar\dot{\psi}_\uparrow(\mathbf{r}) = [\psi_\uparrow(\mathbf{r}), H_{eff}] \\ i\hbar\dot{\psi}_\downarrow(\mathbf{r}) = [\psi_\downarrow(\mathbf{r}), H_{eff}] \end{cases}$

$$\Rightarrow \begin{cases} H_0 u_n(\mathbf{r}) + \Delta(\mathbf{r})v_n(\mathbf{r}) = E_n u_n(\mathbf{r}), \\ H_0^* v_n(\mathbf{r}) - \Delta^*(\mathbf{r})u_n(\mathbf{r}) = -E_n v_n(\mathbf{r}). \end{cases}$$

Bogoliubov-de Gennes (BdG) equations

$$\begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H_0^* \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}.$$

if (u_n, v_n) is a solution with energy E_n, then $(-v_n^*, u_n^*)$ is a solution with energy $-E_n$ (for s-wave SC). Thus, they are orthonormal to each other,

- Orthogonality between eigenstates

$$\begin{cases} \int d^3r\, (u_n^*(\mathbf{r}), v_n^*(\mathbf{r})) \begin{pmatrix} u_{n'}(\mathbf{r}) \\ v_{n'}(\mathbf{r}) \end{pmatrix} = \delta_{nn'}, \\ \int d^3r\, (u_n^*(\mathbf{r}), v_n^*(\mathbf{r})) \begin{pmatrix} -v_{n'}^*(\mathbf{r}) \\ u_{n'}^*(\mathbf{r}) \end{pmatrix} = 0. \end{cases}$$

$$\Rightarrow \begin{cases} \gamma_{n\uparrow} = \int d^3r \left(u_n^*(\mathbf{r})\psi_\uparrow(\mathbf{r}) + v_n^*(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) \right), \\ \gamma_{n\downarrow}^\dagger = \int d^3r \left(-v_n(\mathbf{r})\psi_\uparrow(\mathbf{r}) + u_n(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r}) \right) \end{cases}$$

Note: Particle-hole symmetry: same P as before, and

$$P\mathsf{H}(\mathbf{r}, \mathbf{p})P^{-1} = -\mathsf{H}(\mathbf{r}, -\mathbf{p})$$