Basic notion of Superconductivity

Mechanism of formation of electron pairs due to lattice vibration

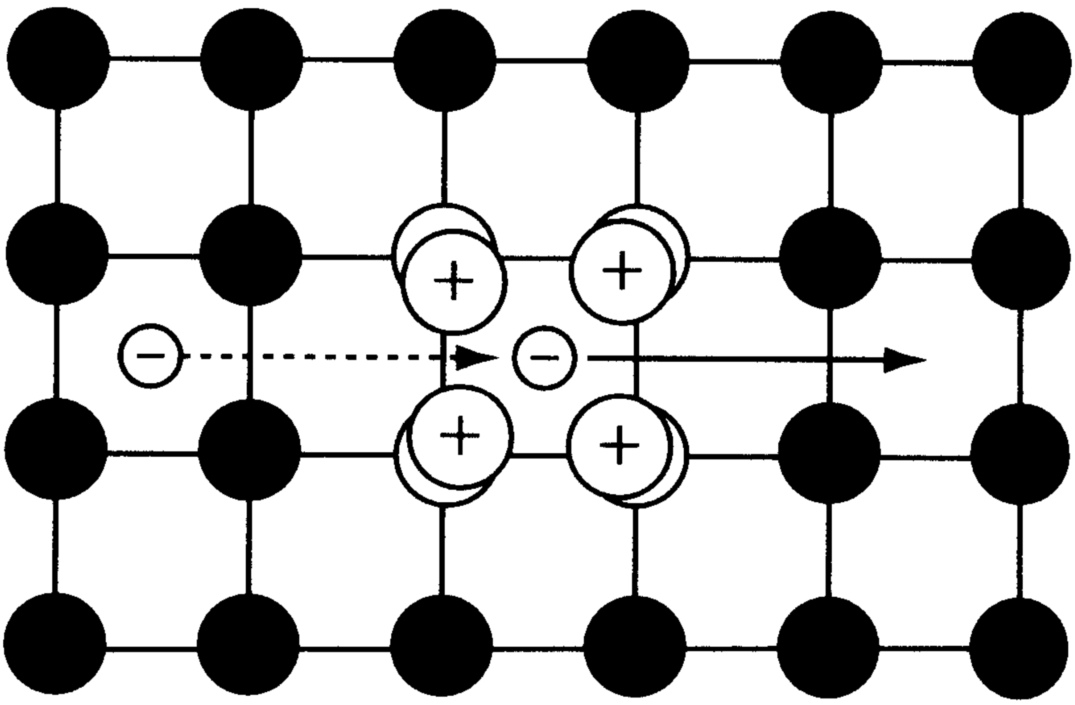
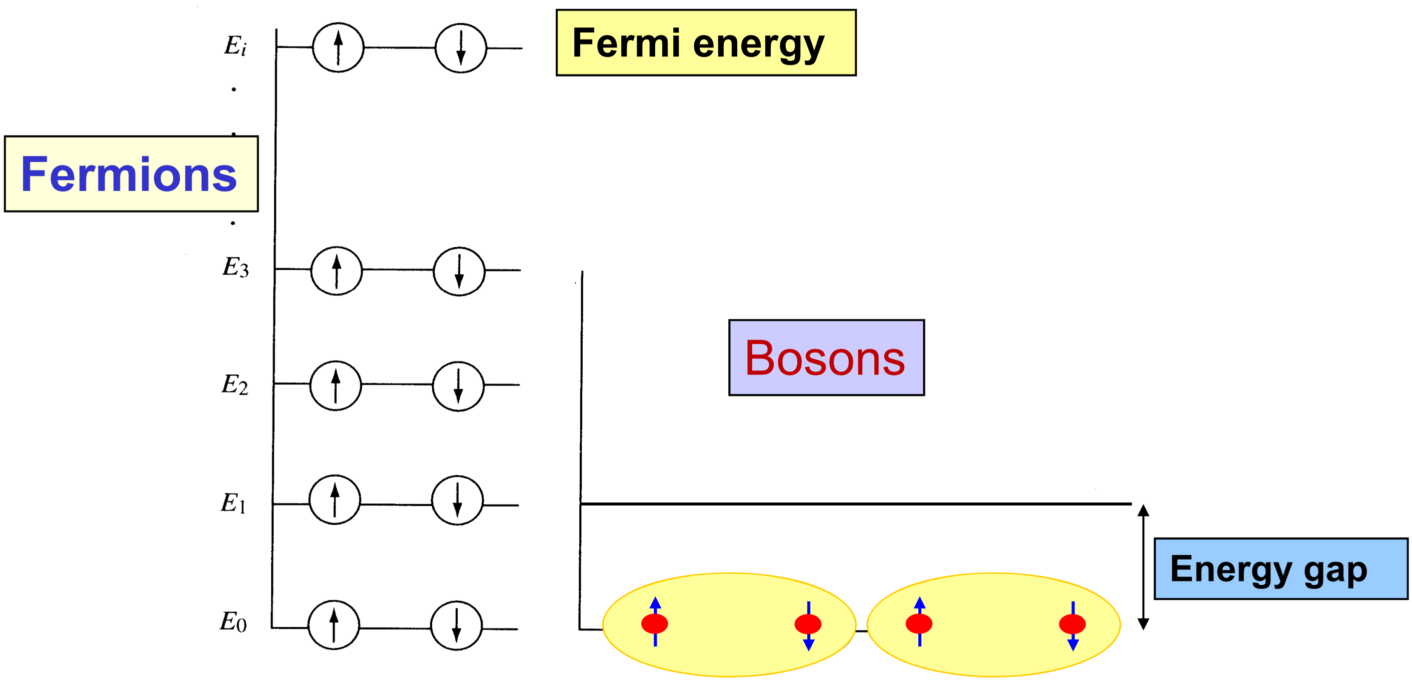


図12　電子間に引力が働く機構の模式図

Concept for Superconductivity



Cooper pairs: $|k\uparrow, -k\downarrow>$

Fermi-Dirac Statistics

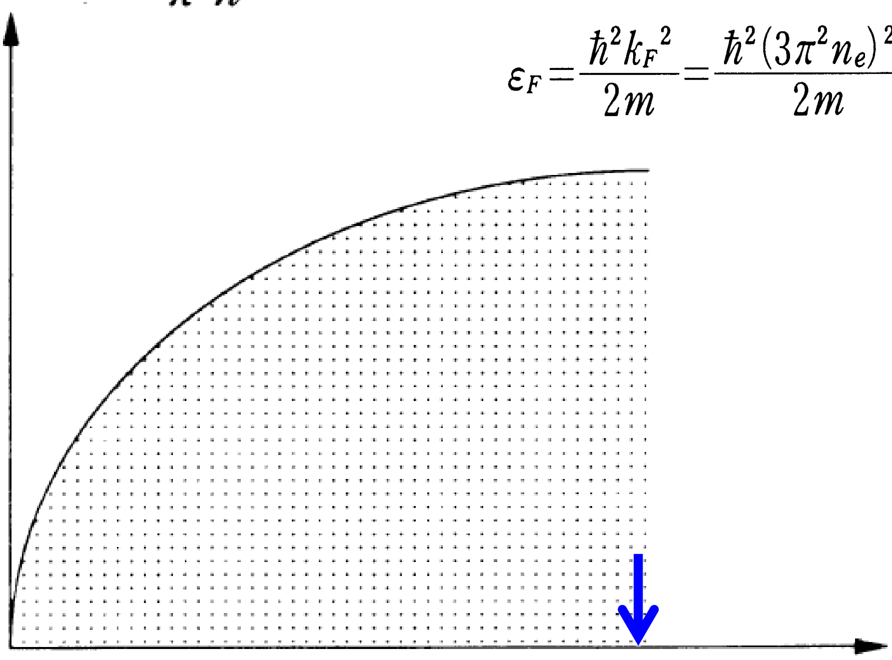
Bose-Einstein Statistics

$$D_{3D}(\varepsilon) = \frac{\sqrt{2}\, m^{3/2}}{\pi^2 \hbar^3}\sqrt{\varepsilon}$$

$$n_e = \frac{2}{(2\pi)^3}\frac{4}{3}\pi k_F{}^3 = \frac{k_F{}^3}{3\pi^2}, \qquad k_F = (3\pi^2 n_e)^{1/3}$$

$$\varepsilon_F = \frac{\hbar^2 k_F{}^2}{2m} = \frac{\hbar^2 (3\pi^2 n_e)^{2/3}}{2m}$$

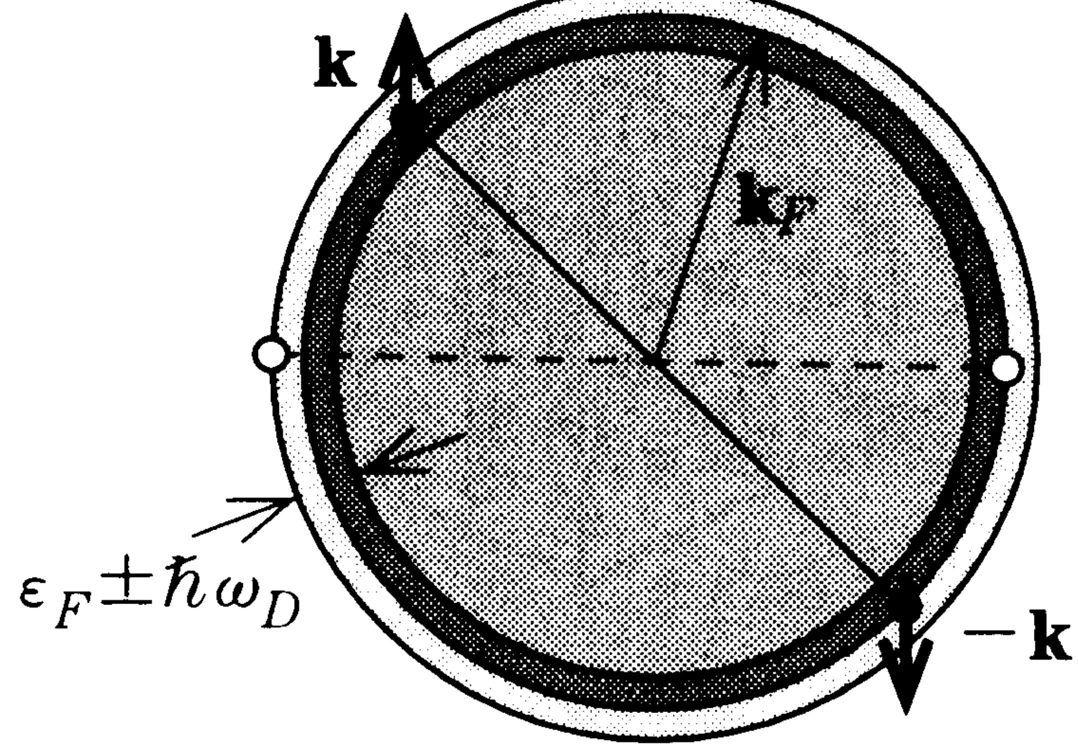
5 ~ 10 eV



E_F : Fermi energy

Electrons density : $n_e = \int_0^{\varepsilon_F} D_{3D}(\varepsilon)\, d\varepsilon = \int_0^{E_F} \frac{\sqrt{2}\, m^{3/2}}{\pi^2 \hbar^3}\sqrt{\varepsilon}\, d\varepsilon = \frac{(2m\varepsilon_F)^{3/2}}{3\pi^2 \hbar^3}$

Provided that attractive interaction works between electrons near the Fermi level, electrons are always bounded making pairs - Cooper pairs -. In order to prove this theorem, we deal with a simple case where two electrons are added on the Fermi sea as illustrated below.



We deal with a following Schrödinger equation for two electrons with attractive potential $V(\mathbf{r}_1, \mathbf{r}_2)$;

$$\left[-\frac{\hbar^2}{2m}(\nabla_1{}^2+\nabla_2{}^2)+V(\mathbf{r}_1,\mathbf{r}_2)\right]\psi(\mathbf{r}_1,\mathbf{r}_2)=E\psi(\mathbf{r}_1,\mathbf{r}_2) \qquad (11.9)$$

In case of $V(\mathbf{r}_1, \mathbf{r}_2) = 0$, the wave function with a lowest energy at zero total momentum is described by the following formula;

$$\psi(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{L^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}_1}\frac{1}{L^{3/2}}e^{-i\mathbf{k}\cdot\mathbf{r}_2}=\frac{1}{L^3}e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \qquad (11.10)$$

Then, for $V(\mathbf{r}_1, \mathbf{r}_2) \neq 0$ a wave function is expressed as follow;

$$\psi(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{L^3}\sum_{|\mathbf{k}|>k_F}A_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \qquad (11.11)$$

Note that since this wave function is symmetric in orbital sector, the spin function is in anti-symmetric spin-singlet state.

Inserting (11.11) into (11.9) and using, $V_{\mathbf{k}}\equiv\int V(\mathbf{r})\,e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}$

$$(E-2\varepsilon_{\mathbf{k}})A_{\mathbf{k}}=\sum_{|\mathbf{k}'|>k_F}V_{\mathbf{k}-\mathbf{k}'}A_{\mathbf{k}'} \qquad (11.12)$$

We can derive this eigen equation.

When the eigen energy in the eq. (11.12) has a solution for E < 2ε_F , two- electron bounded state (Cooper pair) is formed. Provided that $V(\mathbf{r}_1, \mathbf{r}_2)$ is approximated as follows;

$$V_{\mathbf{k}-\mathbf{k}'} = \begin{cases} \text{const} = V < 0 & |\varepsilon_{\mathbf{k}} - \varepsilon_F|,\ |\varepsilon_{\mathbf{k}'} - \varepsilon_F| < \hbar\omega_D \\ 0 & \textbf{otherwise} \end{cases} \qquad (11.13)$$

Here, if the constant attractive interaction V is assumed to be effective only among electrons within energies in the range between the Fermi energy ε_F and the Debye energy $\hbar\omega_D$ which is the highest one of lattice vibration, we obtain the following equation;

$$(E - 2\varepsilon_{\mathbf{k}}) A_{\mathbf{k}} = -|V| \sum_{|\mathbf{k}'| > k_F} A_{\mathbf{k}'} \qquad (11.14)$$

When taking $A \equiv \sum_{|\mathbf{k}'| > k_F} A_{\mathbf{k}'}$, **form** (11.14) **we have** $A_{\mathbf{k}} = -\dfrac{|V|}{E - 2\varepsilon_{\mathbf{k}}} A$ となな

Since $A = A|V| \sum_{0 < (\varepsilon_{\mathbf{k}} - \varepsilon_F) < \hbar\omega_D} \dfrac{1}{2\varepsilon_{\mathbf{k}} - E}$ **, we obtain the following relation**

$$\frac{1}{|V|} = \sum_{\substack{\mathbf{k} \\ 0 < (\varepsilon_{\mathbf{k}} - \varepsilon_F) < \hbar\omega_D}} \frac{1}{2\varepsilon_{\mathbf{k}} - E} \qquad (11.15)$$

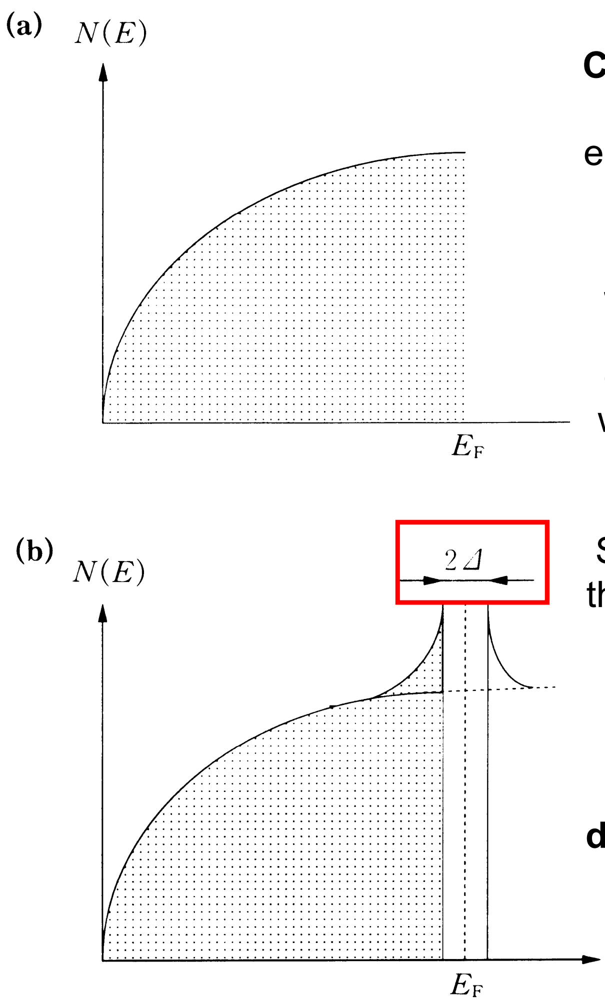
$$\frac{1}{|V|} = \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{1}{2\varepsilon - E} N(\varepsilon)\, d\varepsilon$$

$$\approx N(\varepsilon_F) \int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{1}{2\varepsilon - E}\, d\varepsilon$$

$$= \frac{1}{2} N(\varepsilon_F) \ln\left(\frac{2\varepsilon_F - E + 2\hbar\omega_D}{2\varepsilon_F - E}\right)$$

$N(\varepsilon_F)|V| \ll 1$ **is considered and as a result**

we obtain the eigen energy as $E \approx 2\varepsilon_F - 2\hbar\omega_D e^{-2/N(\varepsilon_F)|V|}$

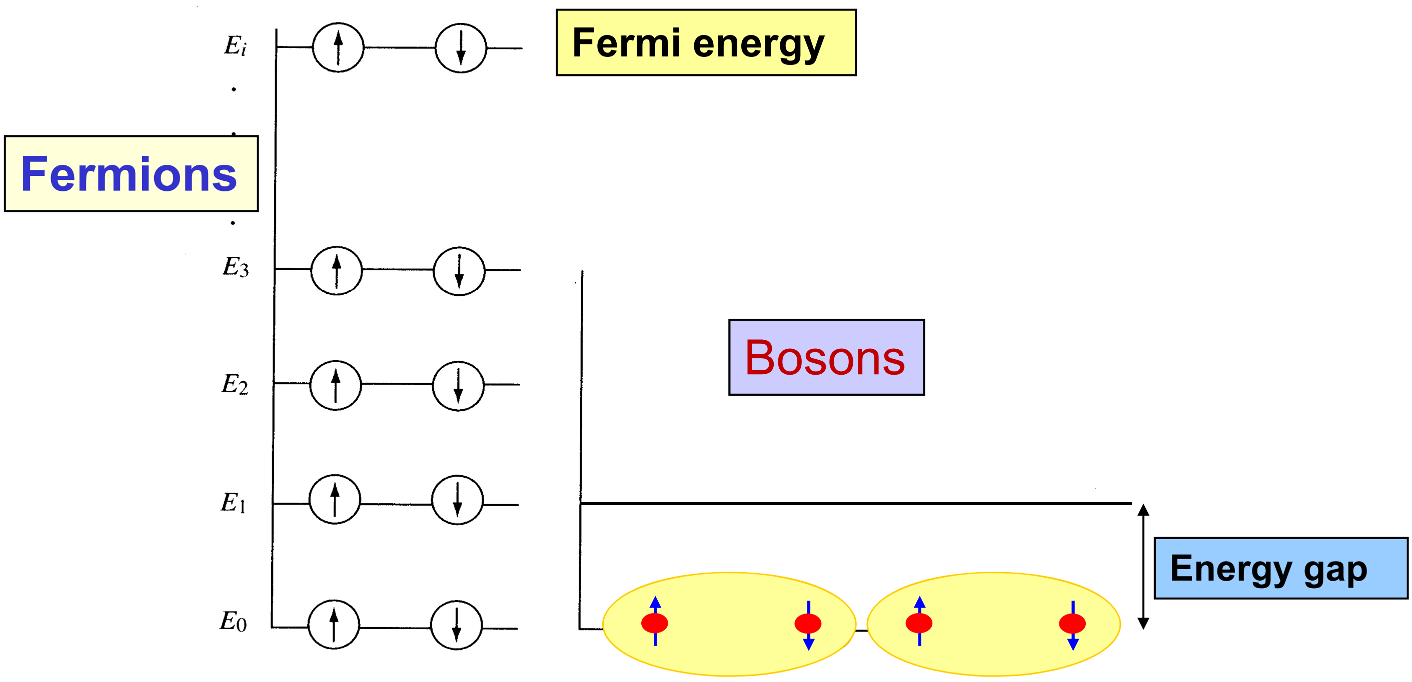


It was proved that electrons near the Fermi surface are bounded making pairs of **(k, ↑)** and **(-k, ↓)** - **Cooper pair-** via the attractive interaction mediated by lattice vibration with highest energy -Debye energy $\hbar\omega_D$. Here the Cooper pair is in the zero total momentum and the spin-singlet state.

Since Cooper pairs are formed by many body of electrons near the Fermi level, these are condensed into **a macroscopic quantum state** which is regarded as a Bose condensation. This outstanding aspect of superconductivity was theoretically clarified by Bardeen, Cooper and Schriefer, and hence this theory is called as BCS theory which is epoch-making event in condensed matter physics in the 20th century.

In this BCS state, **an isotropic energy gap Δ** opens on the Fermi level, yielding **a perfect diamagnetism called Meissner effect** and **zero-resistance effect.**

Concept for Superconductivity



Cooper pairs: |k ↑, - k ↓>

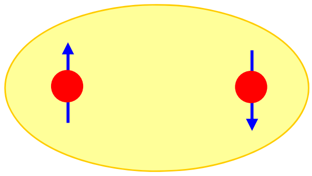
Fermi-Dirac Statistics **Bose-Einstein Statistics**

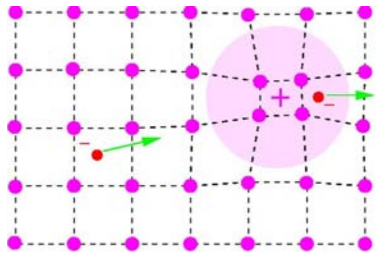
Superconductivity

Conventional superconductivity:

Cooper pair

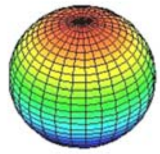
attractive interaction: electron-phonon coupling





s-wave spin singlet

pairing channel: angular momentum l=0 and spin s=0



order parameter: $\Psi(\vec{r}) = |\Psi(\vec{r})| e^{i\phi(\vec{r})}$

broken symmetry: U(1) gauge →
- Meissner-Ochsenfeld-effect (Higgs)
- persistent currents
- flux quantization

Periodic Table for Superconducting Elements

Possible room temperature superconductivity of metallic hydrogen under ultra high pressure exceeding 400 GPa

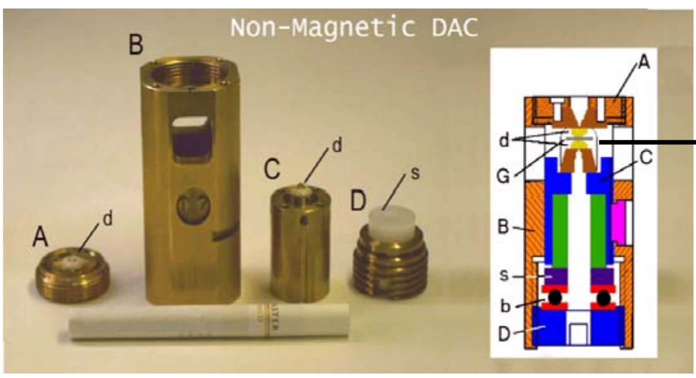
Ambient pressure

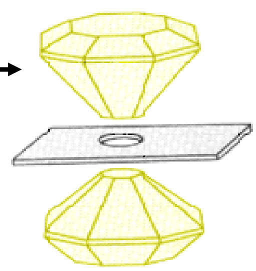
Pressure induced superconducting elements

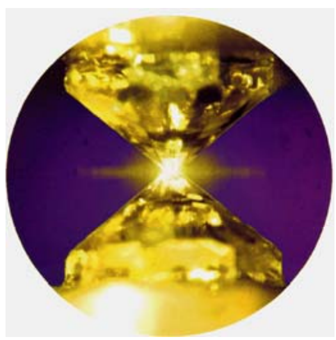
^{1}H																	^{2}He
^{3}Li	^{4}Be											^{5}B	^{6}C	^{7}N	^{8}O	^{9}F	^{10}Ne
^{11}Na	^{12}Mg											^{13}Al	^{14}Si	^{15}P	^{16}S	^{17}Cl	^{18}Ar
^{19}K	^{20}Ca	^{21}Sc	^{22}Ti	^{23}V	^{24}Cr	^{25}Mn	^{26}Fe	^{27}Co	^{28}Ni	^{29}Cu	^{30}Zn	^{31}Ga	^{32}Ge	^{33}As	^{34}Se	^{35}Br	^{36}Kr
^{37}Rb	^{38}Sr	^{39}Y	^{40}Zr	^{41}Nb	^{42}Mo	^{43}Tc	^{44}Ru	^{45}Rh	^{46}Pd	^{47}Ag	^{48}Cd	^{49}In	^{50}Sn	^{51}Sb	^{52}Te	^{53}I	^{54}Xe
^{55}Cs	^{56}Ba	^{57}La	^{72}Hf	^{73}Ta	^{74}W	^{75}Re	^{76}Os	^{77}Ir	^{78}Pt	^{79}Au	^{80}Hg	^{81}Tl	^{82}Pb	^{83}Bi	^{84}Po	^{85}At	^{86}Rn
^{87}Fr	^{88}Ra	^{89}Ac															

Li : K. Shimizu *et al.*, Nature 419 (2002)597.
B : M. I. Eremets *et al.*, Science 293(2001)272.
O : K. Shimizu *et al.*, Nature 393 (1998)767.
Ca : S. Okada *et al.*, J. Phys. Soc. Jpn. **65**, 7 (1996)1924.
Fe : K. Shimizu *et al.*, Nature 412 (2001)316.
S : S. Kometani *et al*,. J. Phys. Soc. Jpn., **66** (1997) 2564.

Experimental technology under ultra high pressure



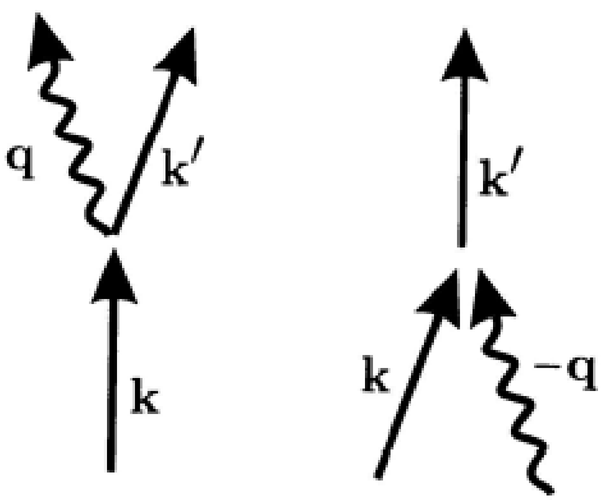




Basic notion for BCS mechanism for Metals

Electron-lattice interaction brings about phonon absorption or emission via mobile electrons.

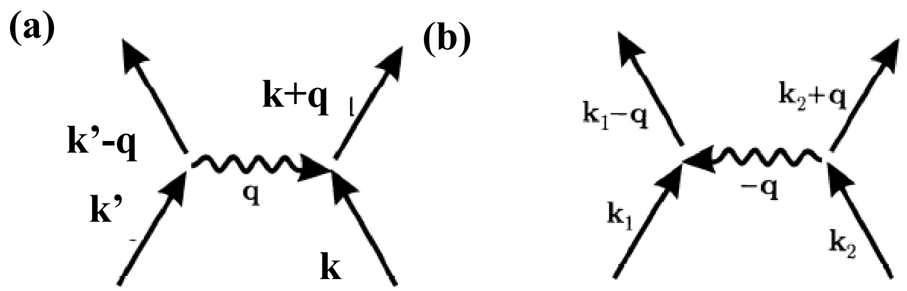
This is the origin of electrical resistance in solid at high temperature.



(a) **(b)**

Electron –phone scattering process

Attractive electron-electron interaction is mediated by the virtual phonon-exchange process.



$$U=\frac{|V_{\mathbf{q}}|^2}{\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}'-\mathbf{q}}-\hbar\omega_{\mathbf{q}}}+\frac{|V_{\mathbf{q}}|^2}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}+\mathbf{q}}-\hbar\omega_{\mathbf{q}}}$$

According to the energy conservation law; $\varepsilon_{\mathbf{k}'}+\varepsilon_{\mathbf{k}}=\varepsilon_{\mathbf{k}'-\mathbf{q}}+\varepsilon_{\mathbf{k}+\mathbf{q}}$

$$U=-\frac{2|V_{\mathbf{q}}|^2(\hbar\omega_{\mathbf{q}})}{(\hbar\omega_{\mathbf{q}})^2-(\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}'-\mathbf{q}})^2}$$

フォノンを媒介とした電子間の引力相互作用（電子-格子相互作用の二次摂動）

状態 k' にある電子が q のフォノンを放出して、$k'-q$ となり、k にある電子が q のフォノンを吸収して、$k+q$ となる過程を考える。この時、エネルギー保存則から、

$$\varepsilon_k+\varepsilon_{k'}=\varepsilon_{k+q}+\varepsilon_{k'-q}$$

電子のフォノン放出やフォノン吸収の相互作用（電子-格子相互作用）を摂動 Hamiltonian (H') として、この二次の摂動過程による系のエネルギー変化 ΔE を計算する。始状態と終状態を形式的に $|\mathrm{i}\rangle$ と $|\mathrm{f}\rangle$ と表して、中間状態 $|m\rangle$ として、図の (a) と (b) を考えれば、

$$\begin{aligned}\Delta E &= \sum_m \frac{\langle \mathrm{f}|H'|m\rangle\langle m|H'|\mathrm{i}\rangle}{E_\mathrm{i}-E_m}\\ &\equiv \sum_m \frac{|M_q|^2}{E_\mathrm{i}-E_m}\end{aligned}$$

ここで、$E_\mathrm{i}=\varepsilon_k+\varepsilon_{k'}$ であり、q のフォノンの放出及び吸収の過程での摂動 Hamiltonian の行列要素を M_q とした。

まず、中間状態として (a) を考えた場合は、$E_{(\mathrm{a})} = \varepsilon_{\boldsymbol{k}'-\boldsymbol{q}} + \varepsilon_{\boldsymbol{k}} + \hbar\omega_{\boldsymbol{q}}$ なので、

$$E_{\mathrm{i}} - E_{(\mathrm{a})} = \varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}'-\boldsymbol{q}} - \hbar\omega_{\boldsymbol{q}}$$

となる。また、中間状態として (b) を考えた場合は、$E_{(\mathrm{b})} = \varepsilon_{\boldsymbol{k}'} + \varepsilon_{\boldsymbol{k}+\boldsymbol{q}} + \hbar\omega_{-\boldsymbol{q}}$ なので、

$$E_{\mathrm{i}} - E_{(\mathrm{b})} = \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \hbar\omega_{-\boldsymbol{q}}$$

となる。従って、ΔE は次のようになる；

$$\begin{aligned}
\Delta E &= |M_{\boldsymbol{q}}|^2 \left(\frac{1}{\varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}'-\boldsymbol{q}} - \hbar\omega_{\boldsymbol{q}}} + \frac{1}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \hbar\omega_{-\boldsymbol{q}}}\right) \\
&= |M_{\boldsymbol{q}}|^2 \left(\frac{1}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} - \hbar\omega_{\boldsymbol{q}}} + \frac{1}{-(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}}) - \hbar\omega_{\boldsymbol{q}}}\right) \\
&= \frac{2|M_{\boldsymbol{q}}|^2 \hbar\omega_{\boldsymbol{q}}}{(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}})^2 - \hbar^2\omega_{\boldsymbol{q}}^2}
\end{aligned}$$

ただし、$\hbar\omega_{-\boldsymbol{q}} = \hbar\omega_{\boldsymbol{q}}$ や、エネルギー保存則を用いた。

2 電子のエネルギー授受の上限の目安は Debye エネルギー $\hbar\omega_{\mathrm{D}}$ であり、$|\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}}| \ll \hbar\omega_{\mathrm{D}}$ なる 2 電子については、

$$\Delta E \simeq -\frac{2|M_{\boldsymbol{q}}|^2}{\hbar\omega_{\boldsymbol{q}}}$$

となり、有効相互作用が引力となり得ることを示す。電子-格子相互作用の考察から、$|q|$ の小さい領域では、実は、$|M_{\boldsymbol{q}}|^2/\hbar\omega_{\boldsymbol{q}}$ が、ほとんど $\boldsymbol{q}$ 依存性を持たないことがわかっている。つまり、この引力相互作用は、等方的な短距離引力であることが示唆される。

What is the origin of metallic superconductivity
－BCS prediction and theory－

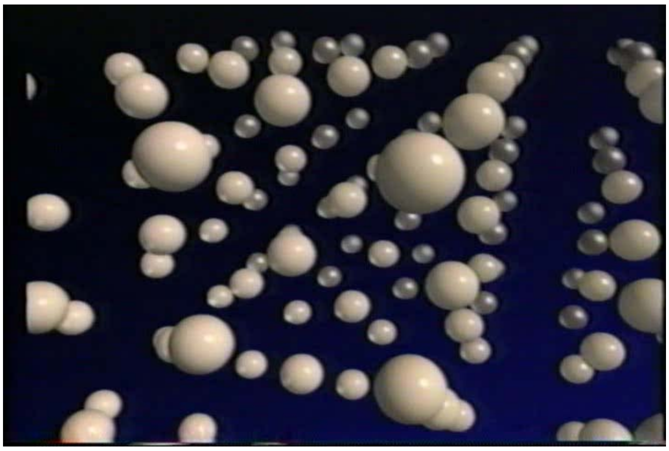
From left side

John **B**ardeen、Leon N. **C**ooper、

J. Robert **S**chrieffer

$$T_c \cong \theta_D exp(-\frac{1}{\lambda})$$

Lattice vibration frequency being higher makes T_c higher

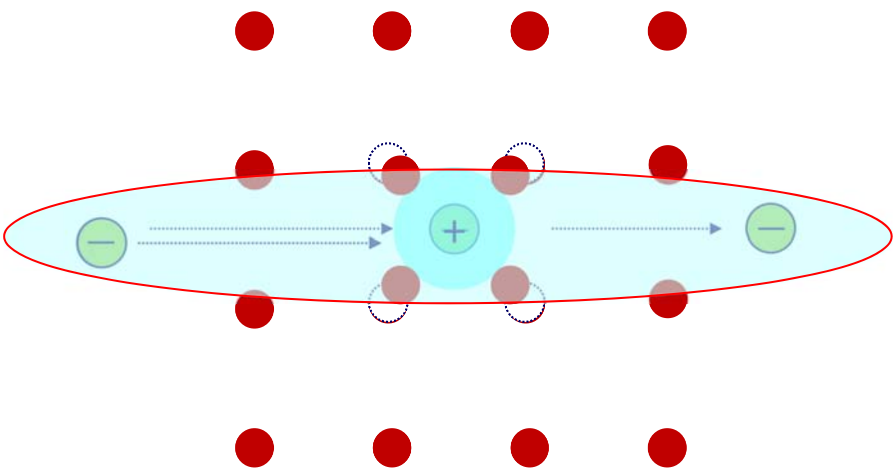


映像：日立サイエンスシリーズ, 超伝導　より

Pictures from Nobelprize.org

BCS Theory

A number of Electron Pairs , which are mediated by the electron-lattice interaction, can coherently propagate without resistance at low temperatures .
This pair is called Cooper pair.



BCS theory predicts the many-body ground state for the superconducting state described by the following wave function as

$$\psi_{\mathrm{BCS}} = \prod_k (u_k + v_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger}) |0\rangle \qquad \textbf{(1)}$$

The BCS Hamiltonian is given by

$$\mathcal{H} = \sum_{k,\sigma} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) c_{k\sigma}^{\dagger} c_{k\sigma} - \sum_{k,k'} V_{kk'} c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} c_{-k'\downarrow} c_{k'\uparrow}$$

Using (1), by minimizing the expectation value of the above BCS Hamiltonian, the parameters u_k and v_k are expressed as follows;

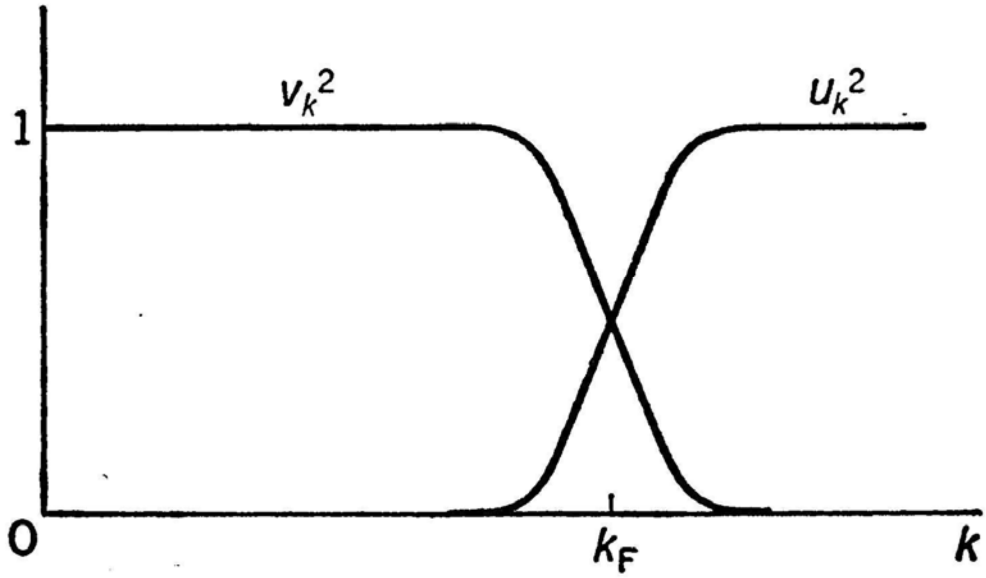
$$u_k^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right), \qquad v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right) \quad \textbf{with} \quad E_k = (\xi_k^2 + |\Delta_k|^2)^{1/2}$$

Here note that $\Delta_k = \langle c_{-k\downarrow} c_{k\uparrow} \rangle$ based ion the mean field approximation and when it is assumed as k-independent, we get the following relations using the density of state at the Fermi Level , N(0) and the Deby frequency, ω_D .

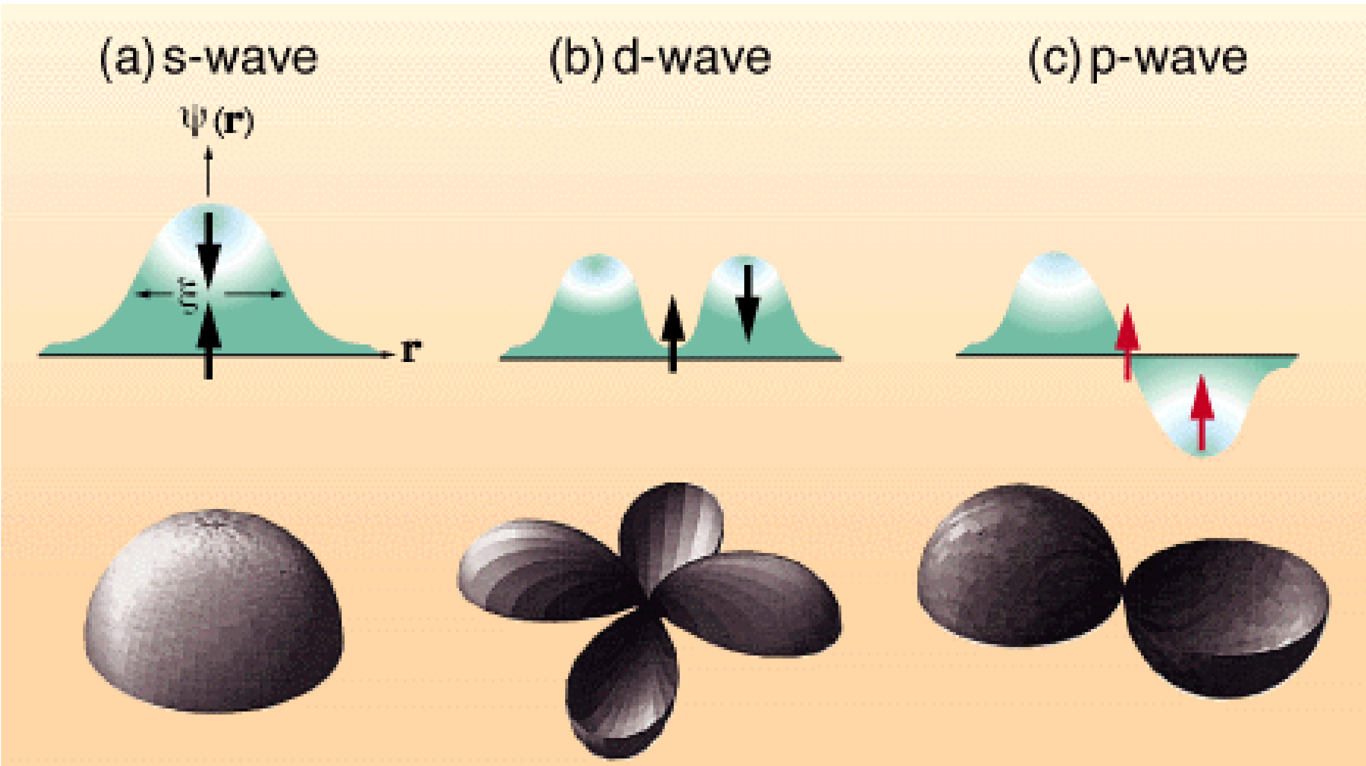
$$1 = \frac{1}{2} N(0)\, V \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{1}{\sqrt{\xi^2 + \Delta^2}}\, d\xi \qquad \Delta = \frac{\hbar\omega_D}{\sinh\left(\frac{1}{N(0)V}\right)} \approx 2\hbar\omega_D \exp\left(-\frac{1}{N(0)V}\right)$$

$$|\Delta| = v_0 {\sum_k}' \frac{|\Delta|}{2E_k} \tanh\left(\frac{E_k(T)}{2k_B T}\right)$$

$$\psi_{\mathrm{BCS}} = \prod_k (u_k + v_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger}) |0\rangle$$



Possible SC order parameters and their spin-state



BCS SC

High-T_c oxides

$CeCu_2Si_2$ UPd_2Al_3, $CeRIn_5$

UPt_3

Sr_2RuO_4

A Route to enhance T_c

The BSC theory based on the electron-lattice vibration interaction derived the formula for the onset of superconductivity given by

$$T_c \sim \hbar\omega_0 \, exp\, [\, -1/\, N(0)V\,]$$

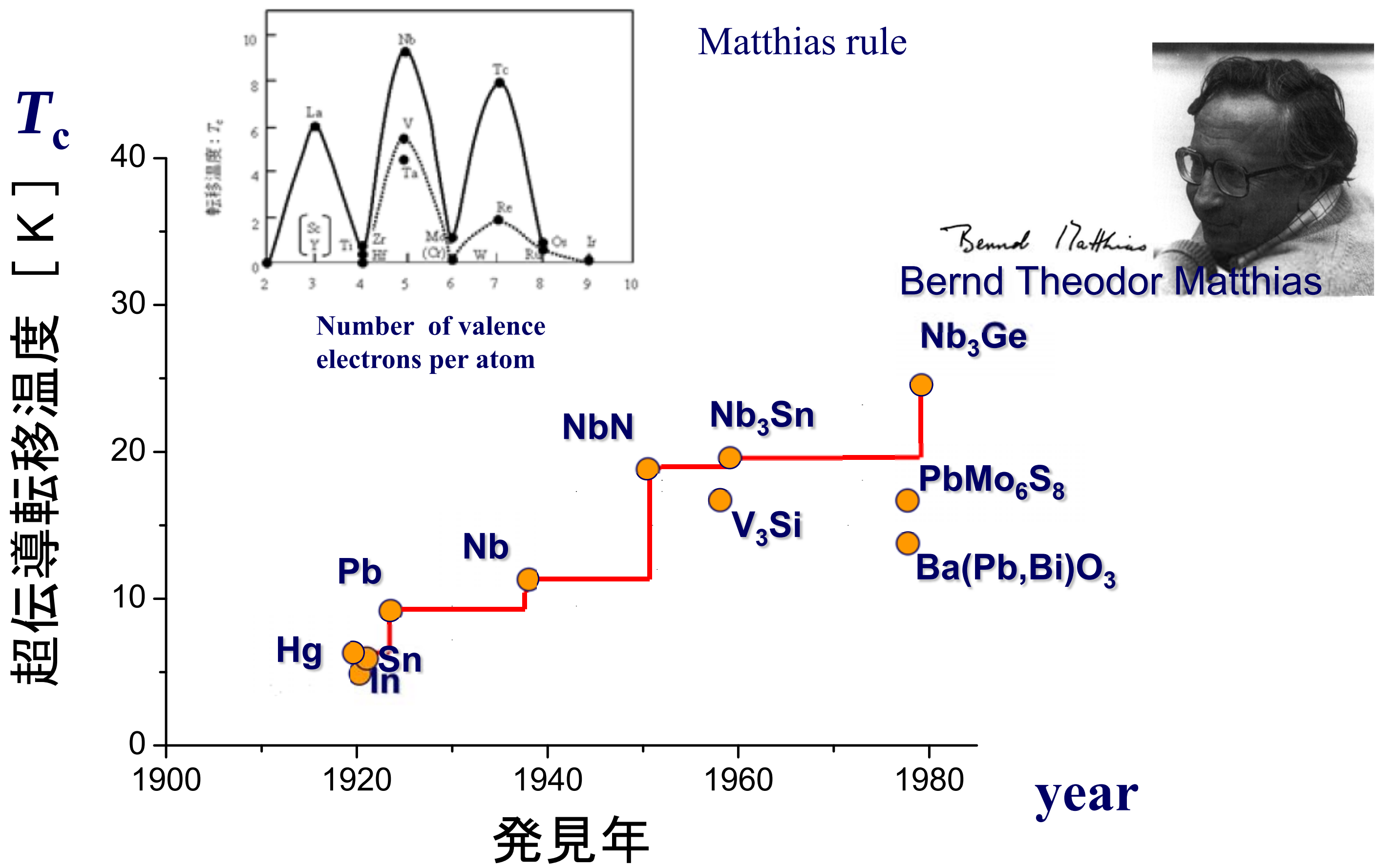
In order to enhance T_c, we may look for materials in which either Θ_D or $N(0)$ or V is larger than existing superconductors.

However, even if $\hbar\omega_0 = \Theta_D$ becomes larger, T_c is not always increased more as evidenced from the following data

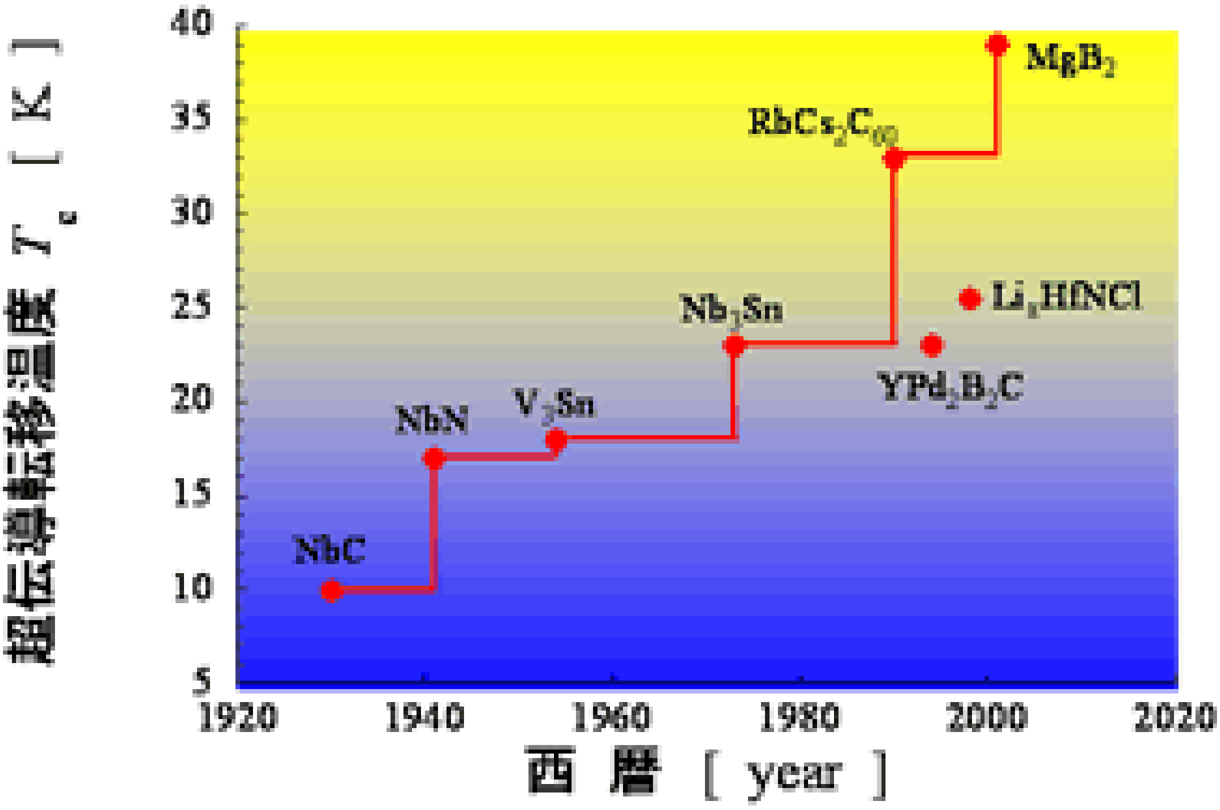
表 5-1　超伝導元素の臨界温度とデバイ温度.

	臨界温度(K)	デバイ温度(K)
Be	0.03	1390
Al	1.16	428
Ga	1.08	325
Sn	3.72	200
Pb	7.19	105

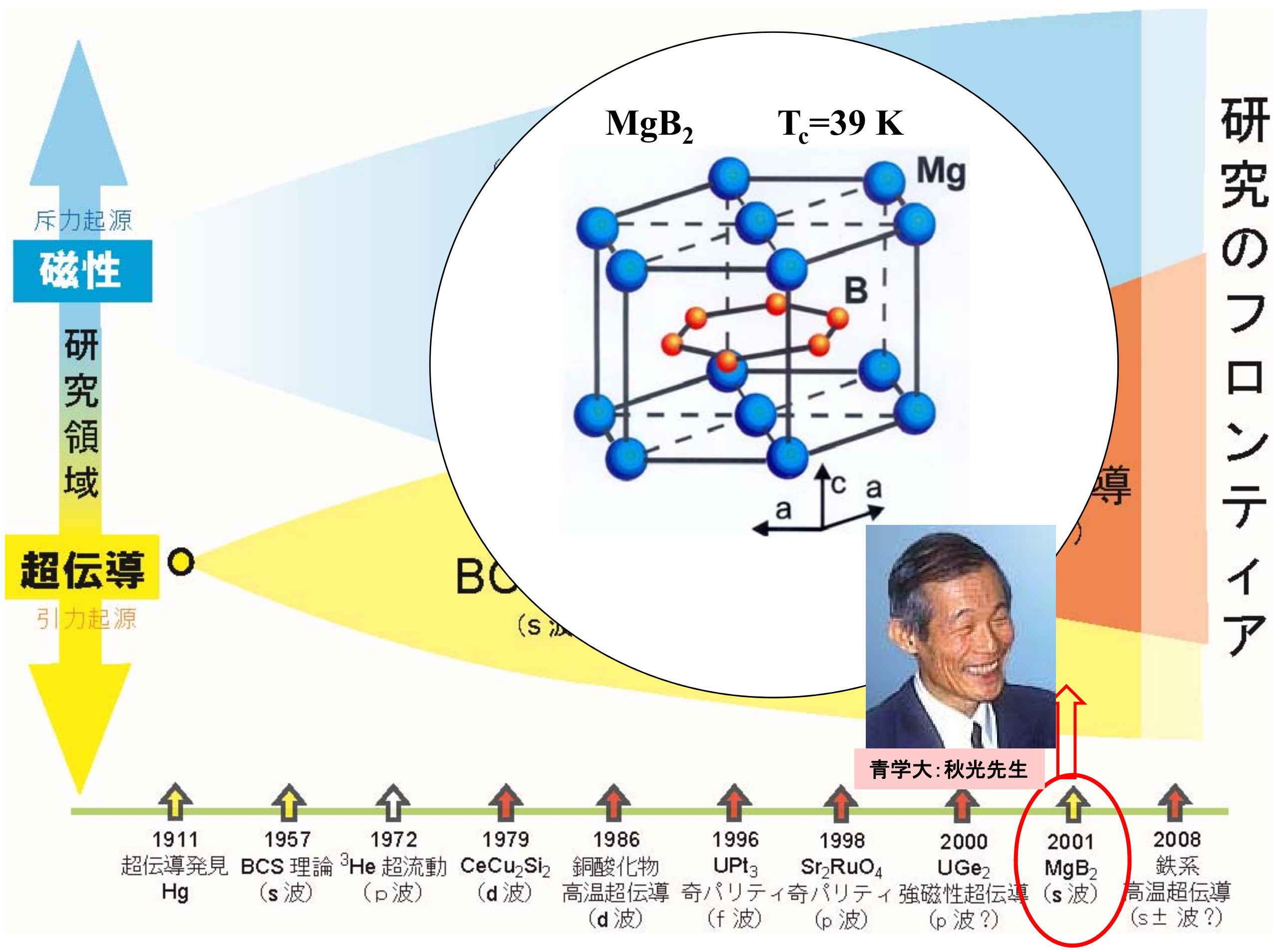
What about increasing $N(0)$ term ? ?



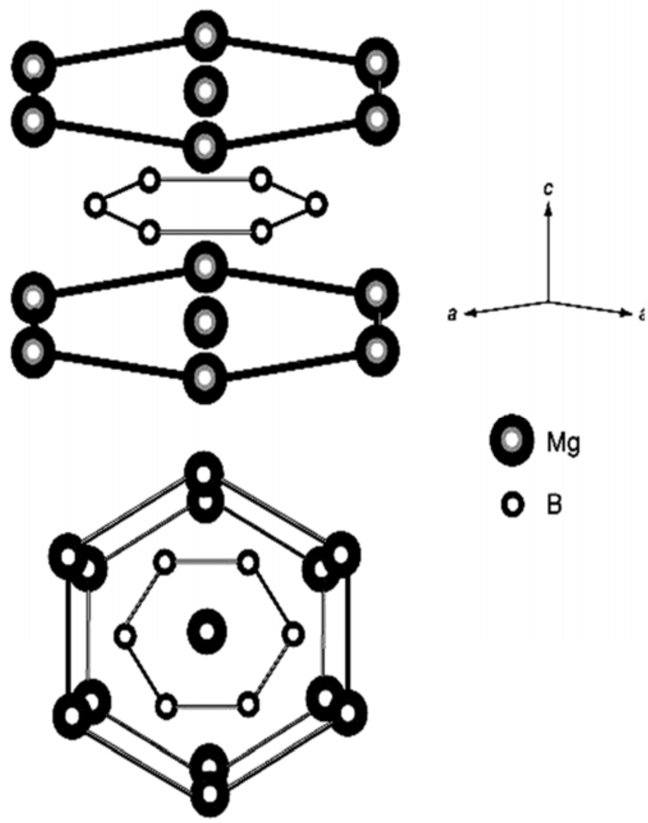
History of T_C for BCS superconductors

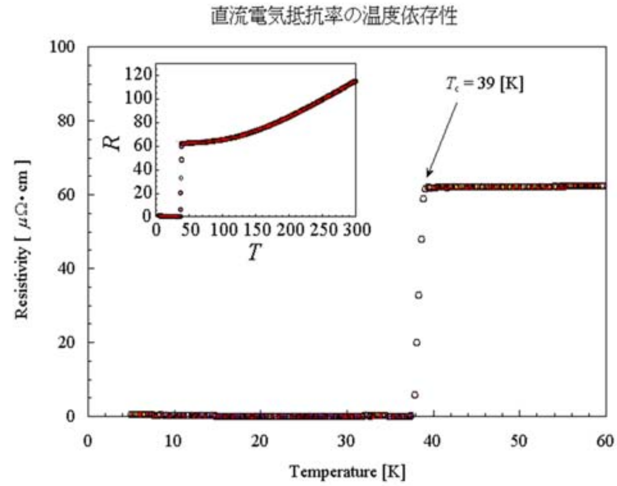


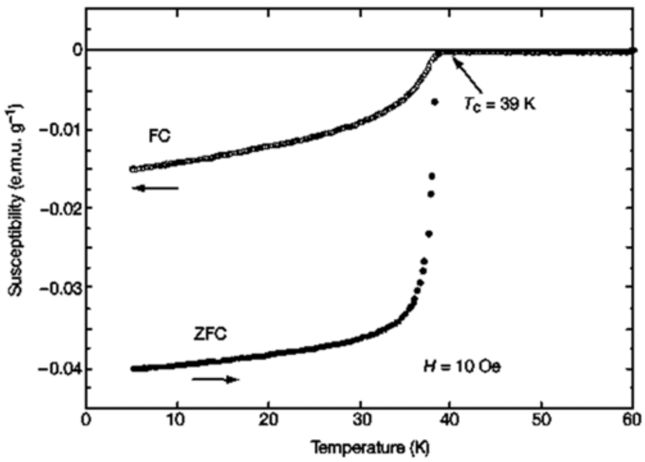
Discovery of MgB$_2$ with a highest T_c =39 K due to the BCS mechanisim



MgB_2





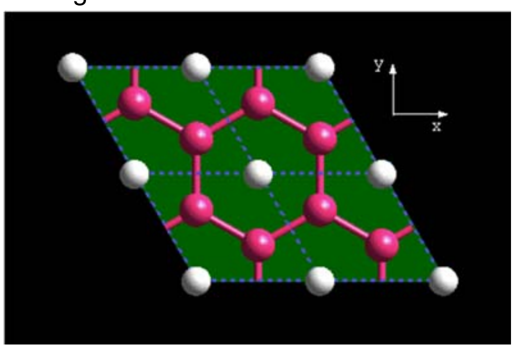


High-frequency optical mode of Boron lattice vibration

Y. Kong *et al*., PRB **64**, 020501(R) (2001).

Light mass (B)
2D honey-comb lattice
reasonable density of states
are the causes to enhance
the highest T_C =39 K

E_{2g}モード



A. Y. Liu *et al*., PRL **87**, 087005 (2001).

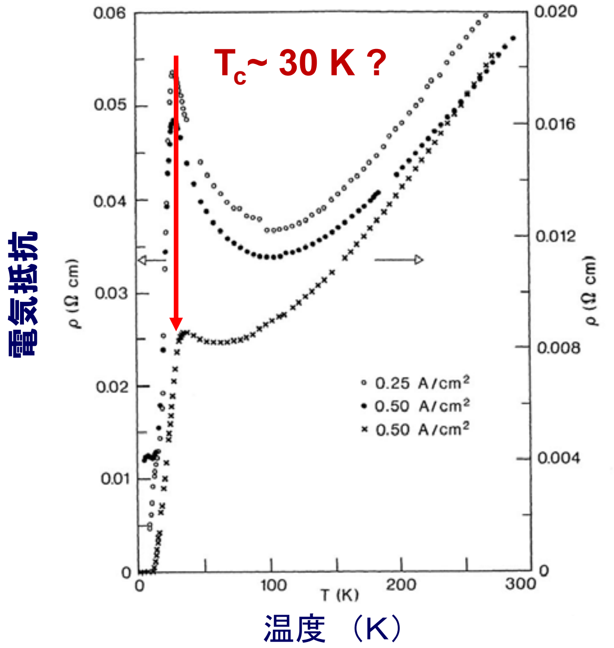
optical E_{2g} mode is strongly coupled with electron

Cal. ω_D= 670〜860K
λ= 0.73〜1

NMR : ω〜700K
λ〜0.87

Cupper Oxides High-T_C superconductor

"Possible High-T_c Superconductivity in the Ba-La-Cu-O System"



J. G. Bednorz and K. A. Muller, Z. Physik B64, 189 (1986)

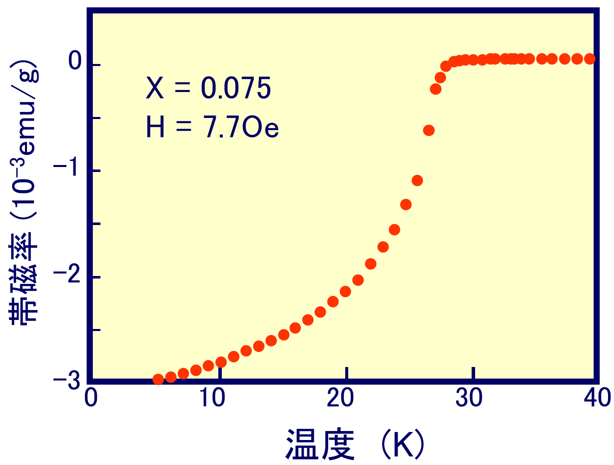
Muller

1987 Novel Prize in Physics

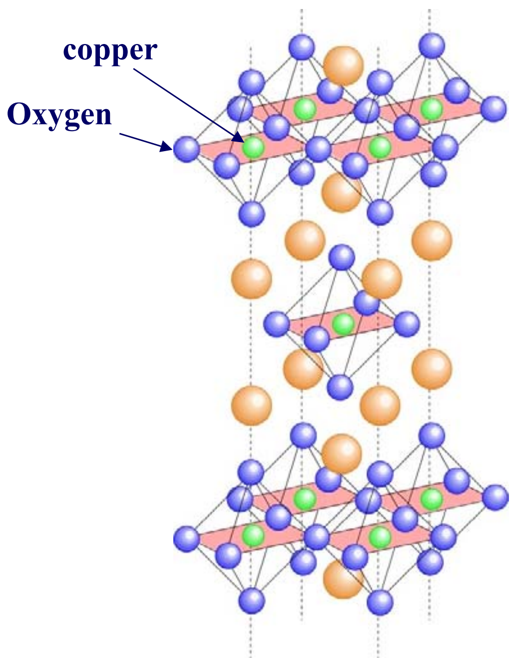
Bednorz

"Possible… " ⟶ Evidence ！

Confirmation of the onset of high-Tc superconductivity and the lattice structure



Meissner effect

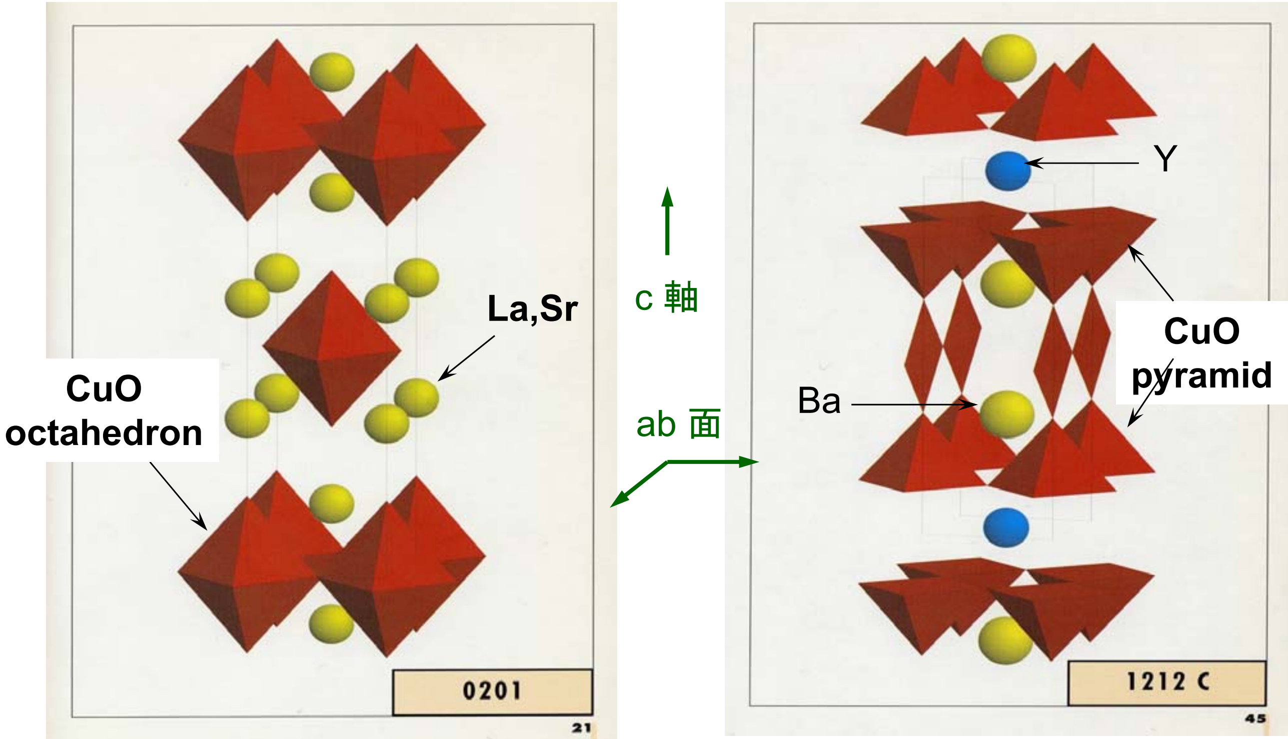


Layered perovskite oxide
CuO_2 plane

High-T_c Copper Oxides superconductors

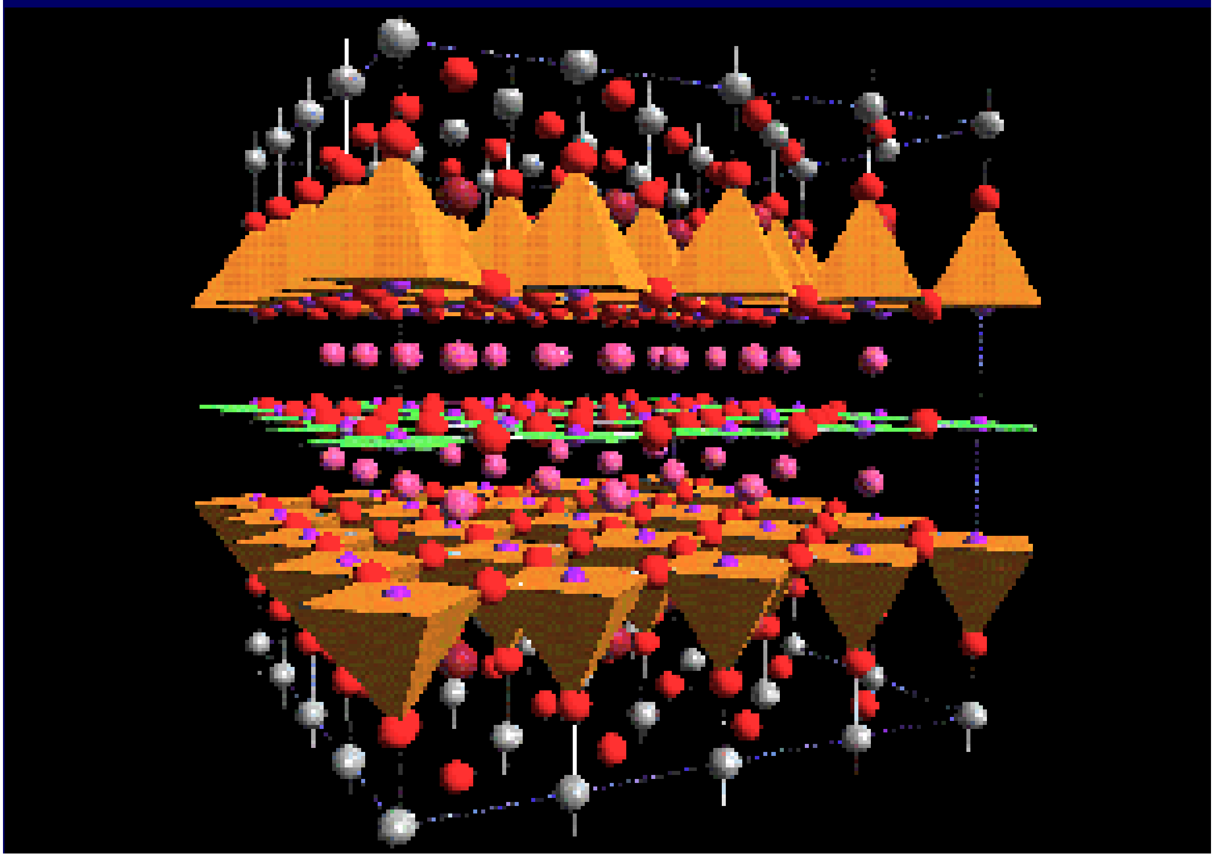
$La_{2-x}Sr_xCuO_4$ 、T_C〜40K

$YBa_2Cu_3O_{7-x}$ 、T_C〜90K



$HgBa_2Ca_2Cu_3O_{6-y}$

A highest T_c ~ 163 K under pressure



Problem 8. We consider a system with electron pairs of R. The superconducting (SC) model Hamiltonian is described as the sum of kinetic term (H_0) and an attractive potential term (V) as follow;

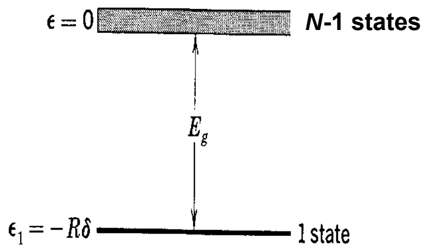
$H = H_0 + V$ where the respective matrix elements are defined as follows;

$$< \{k_i \uparrow, -k_i \downarrow| H_0 | k_i \uparrow, -k_i \downarrow> = 0 \qquad U_{ij} = \langle \{\boldsymbol{k}_i \uparrow,\ -\boldsymbol{k}_i \downarrow\} | V | \{\boldsymbol{k}_j \uparrow,\ -\boldsymbol{k}_j \downarrow\} \rangle = -\delta$$

A trial wave function consisting of the Cooper pairs for the above SC model Hamiltonian is given by the total sum of the wave function of electron pair as follow;

$$\Psi_g = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} c_i \{\boldsymbol{k}_i \uparrow,\ -\boldsymbol{k}_i \downarrow\}$$. Then, from

hint !



$$H\Psi_g = E\ \Psi_g$$

write down the matrix of this Hamiltonian. Furthermore, using the following theorems for the N-roots (E_1, E_2, ------, E_N) on this obtained matrix with the equations of

$$\sum_{i}^{N} E_i = -\delta N$$

$$\sum_{i}^{N} E_i^{\,2} = (\delta N)^2$$

Answer an eigen energy of this model BCS state and its eigen function.

レポート8

***N*個のクーパー対がある系を考える。系のハミルトニアンは、運動エネルギー(H_0)と引力相互作用（V)の和として**

$$H = H_0 + V$$

$$< \{k_i \uparrow, -k_i \downarrow| H_0 | k_i \uparrow, -k_i \downarrow> = 0$$

$$U_{ij} = \langle \{\boldsymbol{k}_i \uparrow,\ -\boldsymbol{k}_i \downarrow\} | V | \{\boldsymbol{k}_j \uparrow,\ -\boldsymbol{k}_j \downarrow\} \rangle = -\delta$$

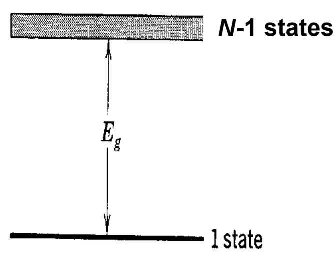
と書けるとする。この系の永年方程式は

$$\begin{vmatrix} -\delta-E & -\delta & \cdots & -\delta \\ -\delta & -\delta-E & \cdots & -\delta \\ \vdots & \vdots & & \vdots \\ -\delta & -\delta & \cdots & -\delta-E \end{vmatrix} = 0$$ **,となる。**

この行列式の *N* 個の根に関する定理:	$\sum_{i}^{N} E_i = -\delta N$ $\sum_{i}^{N} E_i^{\,2} = (\delta N)^2$

を使って、この系の基底状態（BCS状態）の固有エネルギーE_gをもとめ、固有関数は

$$\Psi_g = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \{\boldsymbol{k}_i \uparrow,\ -\boldsymbol{k}_i \downarrow\}$$



となることを示せ。

おわり