

SUPERCONDUCTIVITY

Let us try to make a simplified model to describe the theory of superconductivity, formulated by Bardeen, Cooper, and Schrieffer (BCS). The basic idea is that if we take our free gas of electrons and add a weak interaction among electrons, we can have the formation of Cooper pairs, i.e., pairs of electrons in a state with total spin 0 or 1. That makes my Cooper pair a boson; as such, Cooper pairs can undergo Bose-Einstein condensation and show very interesting features.

Let us start with a system of electrons in its ground state at temperature $T=0$. All energy levels up to E_F are full. In technical term, the Fermi sea is completely filled. Let us now add two electrons; we want to see if there is a bound state of two electrons added to the Fermi sea (i.e., their energy, if I look at them separately, will have to be $> E_F$).

We need to find a solution to the Schrodinger equation for two identical fermions:

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

derivative w.r.t. r, θ, ϕ

Since the two electrons are identical fermions, we have: $\psi(\vec{r}_1, \vec{r}_2) = -\psi(\vec{r}_2, \vec{r}_1)$. Each electron is free, but confined within a box, with periodic boundary conditions: the single-particle solution will be in the form $e^{+i\vec{k} \cdot \vec{r}}$.

Hence (let us treat $V(\vec{r}_1, \vec{r}_2)$ as a small perturbation):

$$\psi(\vec{r}_1, \vec{r}_2) \propto e^{+i\vec{k} \cdot \vec{r}_1} \cdot e^{-i\vec{k} \cdot \vec{r}_2} \quad |\vec{k}| > k_F, \text{ electrons are added to a filled sea}$$

k_F is defined using the Fermi energy: $E_F = \frac{\hbar^2 k_F^2}{2m}$.

Note the form of $\psi(\vec{r}_1, \vec{r}_2)$: We are looking for a state with minimal energy: this is achieved when the two electrons have equal and opposite

momentum (so that their center of mass is at rest). Let us now add spin to our wavefunction. Since the electrons are identical fermions, we need the wavefunction, a product of a space part and a spin part, to be anti-symmetric for particle exchange. I have two possibilities:

$$\Psi_{SA}(1,2) = \cos(\vec{k} \cdot \vec{r}) |00\rangle \quad \text{space symmetric} \cdot \text{spin anti-symmetric}$$

$$\Psi_{AS}(1,2) = \sin(\vec{k} \cdot \vec{r}) \begin{cases} |11\rangle \\ |10\rangle \\ |1-1\rangle \end{cases} \quad \text{space anti-symmetric} \cdot \text{spin symmetric}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \quad |S S_z\rangle \quad \vec{S} = \vec{S}_1 + \vec{S}_2$$

If there is a small attractive force between electrons (the potential V we treated as a perturbation), Ψ_{SA} is favored: remember that in a symmetric space ^{wave}function, the two particles stay closer to each other. We can now write the generic wavefunction for a two-electron states considering that any pair of states

$(\vec{k}, -\vec{k})$ are allowed, when $|\vec{k}| > k_F$. Let us write our solution as a series:

$$\Psi(\vec{r}_1, \vec{r}_2) = \sum_{k > k_F} g_k \cos(\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)) |00\rangle$$

\leftarrow momentum of electron 1 \leftarrow momentum of electron 2
 \searrow weighing function: depends on $|\vec{k}|$, not on \vec{k}
 \searrow sum over all momentum eigenstates outside Fermi sphere.

Let us put this guess into Schrodinger equation. We obtain:

$$(E - 2E_k) g_k = \sum_{k'} g_{k'} V_{k,k'} \quad \text{where } V_{k,k'} = \int d^3\vec{r} V(\vec{r}) e^{-i(\vec{k}-\vec{k}') \cdot \vec{r}}$$

and $E_k = \hbar^2 k^2 / 2m$

It is easy to see that the $2E_k$ piece comes from:

$$\left(-\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 \right) \left(\sum g_k e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} |00\rangle \right)$$

It is a bit more complicated to find the other term, with $V_{k,k'}$; quite a bit of manipulation is needed.

Let us focus on the physics. We need an attractive potential, and some explanation for its origin. BCS proposed a very simple potential:

$$V_{\vec{k}, \vec{k}'}^{\text{Cooper}} = \begin{cases} -V_0 & \text{when } E_F < E_{\vec{k}} < E_F + \hbar\omega_c \\ 0 & \text{otherwise} \end{cases}$$

where $\hbar\omega_c$ is a cut-off energy, away from E_F . It was shown by Frohlich that electrons can attract each other through an interaction well-tuned with the vibrations of the positive ion lattice (phonons); the approximate potential is the one above. This potential favors pairings that involve scattering from $(\vec{k}, -\vec{k})$ to $(\vec{k}', -\vec{k}')$ states, where both \vec{k} and \vec{k}' are within a thin shell of thickness $\hbar\omega_c$ on the Fermi surface. The scale of the thickness of this shell is given by $\hbar\omega_c$, which is the characteristic energy of lattice vibration: the Debye energy.

We can now solve our equation; in the approximation $N(E_F) \cdot V \ll 1$ (where $N(E_F)$ is the density of states at the Fermi energy), we obtain:

$$E \approx 2E_F - 2\hbar\omega_c e^{-2/N(E_F) \cdot V}$$

This is smaller than $2E_F$, the energy of the two free electrons: it is a BOUND STATE, which we call a COOPER PAIR. Let us note that this bound state exists, regardless of how weak the potential V is. Let us also note that the binding energy is proportional to $\hbar\omega_c$, which is characterized by the Debye temperature T_D .

T_D also depends on $1/\sqrt{M}$ (imagine the crystal lattice as an harmonic oscillator). This model predicts that the transition temperature to superconducting mode scales like $T_c \propto 1/\sqrt{M}$, in other words $T_c \cdot \sqrt{M} = \text{constant}$.

This relation has been proven experimentally using metals made of different isotopes (hence it is called "the isotope effect") and constitutes a fundamental success of the BCS theory.

EXTRA: Skipped calculations

Schrodinger equation with ansatz $\psi(1,2) = \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$:

$$\left(-\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 + V(\vec{r}_1 - \vec{r}_2)\right) \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} = E \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

potential must be symmetric for particle exchange: it can't tell which is which

$$\left(-\frac{\hbar^2}{2m} \nabla_1^2\right) \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} = \sum_{\vec{k}} -\frac{\hbar^2}{2m} g_{\vec{k}} \nabla_1^2 e^{i\vec{k}\cdot\vec{r}} = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

same for ∇_2^2 :

$$\nabla_2^2 e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)} = (-i\vec{k}) \cdot (-i\vec{k}) = k^2$$

$$\sum_{\vec{k}} V(\vec{r}_1 - \vec{r}_2) g_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}_1 - \vec{r}_2)} = \sum_{\vec{k}} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{r}'} V_{\vec{r}'} e^{i\vec{r}'\cdot\vec{r}} =$$

$$= \sum_{\vec{r}'} \sum_{\vec{k}} g_{\vec{k}} V_{\vec{r}'} e^{i(\vec{k} + \vec{r}')\cdot\vec{r}} = \sum_{\vec{k}'} \sum_{\vec{r}''} g_{\vec{k}'} V_{\vec{r}''} e^{i\vec{k}'\cdot\vec{r}} =$$

$$= \sum_{\vec{k}'} \sum_{\vec{r}'} g_{\vec{k}'} e^{i\vec{k}'\cdot\vec{r}} V_{\vec{r}-\vec{r}'}$$

where $V(\vec{r}) = \sum_{\vec{r}'} V_{\vec{r}'} e^{i\vec{r}'\cdot\vec{r}}$ means $V_{\vec{r}-\vec{r}'} = \int d^3\vec{r} V(\vec{r}) e^{-i(\vec{r}-\vec{r}')\cdot\vec{r}}$

rename: $\vec{k} \rightarrow \vec{k}'$
 $\vec{k}'' \rightarrow \vec{k}$

Putting everything together:

$$\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \sum_{\vec{k}} \sum_{\vec{r}'} g_{\vec{k}'} V_{\vec{r}-\vec{r}'} e^{i\vec{k}\cdot\vec{r}} = \sum_{\vec{k}} E g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

each term in the sum needs to match the corresponding terms, the $e^{i\vec{k}\cdot\vec{r}}$ terms can be simplified, and we finally obtain:

$$2 \underbrace{\frac{\hbar^2 k^2}{2m}}_{E_{\vec{k}}} g_{\vec{k}} + \sum_{\vec{r}'} g_{\vec{k}'} V_{\vec{r}-\vec{r}'} = E g_{\vec{k}}$$

$$\Rightarrow (E - 2E_{\vec{k}}) g_{\vec{k}} = \sum_{\vec{r}'} g_{\vec{k}'} V_{\vec{r}-\vec{r}'} \quad V_{\vec{r}-\vec{r}'} = \int d^3\vec{r} V(\vec{r}) e^{-i(\vec{r}-\vec{r}')\cdot\vec{r}}$$

Let us now (try and) solve the equation:

$$(E - 2E_k)g_k = \sum_{\vec{k}'} g_{\vec{k}'} V_{\vec{k}, \vec{k}'}$$

The original BCS theory approximates the potential as: $V_{\vec{k}, \vec{k}'} \approx -V_0$, with an energy cutoff $E_F + \hbar\omega_D$.

Then:

$$(E - 2E_k)g_k = -V_0 \sum_{\vec{k}'} g_{\vec{k}'}$$

$$\frac{1}{V_0} g_k = \frac{1}{2E_k - E} \sum_{\vec{k}'} g_{\vec{k}'}$$

$$\sum_{\vec{k}} \frac{1}{V_0} g_k = \sum_{\vec{k}} \frac{1}{2E_k - E} \cdot \sum_{\vec{k}'} g_{\vec{k}'} \rightarrow \sum_{\vec{k}} g_k \text{ simplifies on both sides}$$

$$\frac{1}{V_0} = \sum_{\vec{k}} \frac{1}{2E_k - E}$$

Let us now replace the sum over \vec{k} with an integral over E_k . We need to keep in mind that $\sum_{\vec{k}}$ is a sum over states, hence I need to add a density of states as a function of E_k when I introduce an integral. In short:

$$\sum_{\vec{k}} \rightarrow N(E_F) \int_{E_F}^{E_F + \hbar\omega_D} dE_k \quad \text{where } N(E) = \text{density of states at the Fermi surface} \\ \propto \left. \frac{dm}{dE_k} \right|_{E_k = E_F}$$

We finally obtain:

$$\frac{1}{V_0} = N(E_F) \int_{E_F}^{E_F + \hbar\omega_D} \frac{dE_k}{2E_k - E} = \frac{N(E_F)}{2} \ln \left(\frac{2E_F + 2\hbar\omega_D - E}{2E_F - E} \right)$$

also this piece is ≈ 0 , but I cannot remove it because it is the only term with $\hbar\omega_D$

If $N(E_F) \cdot V_0 \ll 1$, we obtain, approximately:

$$e^{\frac{2}{N(E_F)V_0}} = \frac{2E_F + 2\hbar\omega_D - E}{2E_F - E}$$

$$2E_F - E = 2E_F e^{-\frac{2}{N(E_F)V_0}} + 2\hbar\omega_D e^{-\frac{2}{N(E_F)V_0}} - E e^{-\frac{2}{N(E_F)V_0}}$$

$V_0 \leftarrow$ compare with term on left side of equation $\rightarrow 2$

$$\Rightarrow E \approx 2E_F - 2\hbar\omega_D e^{-\frac{2}{N(E_F)V_0}}$$