Laboratori Nazionali di Frascati

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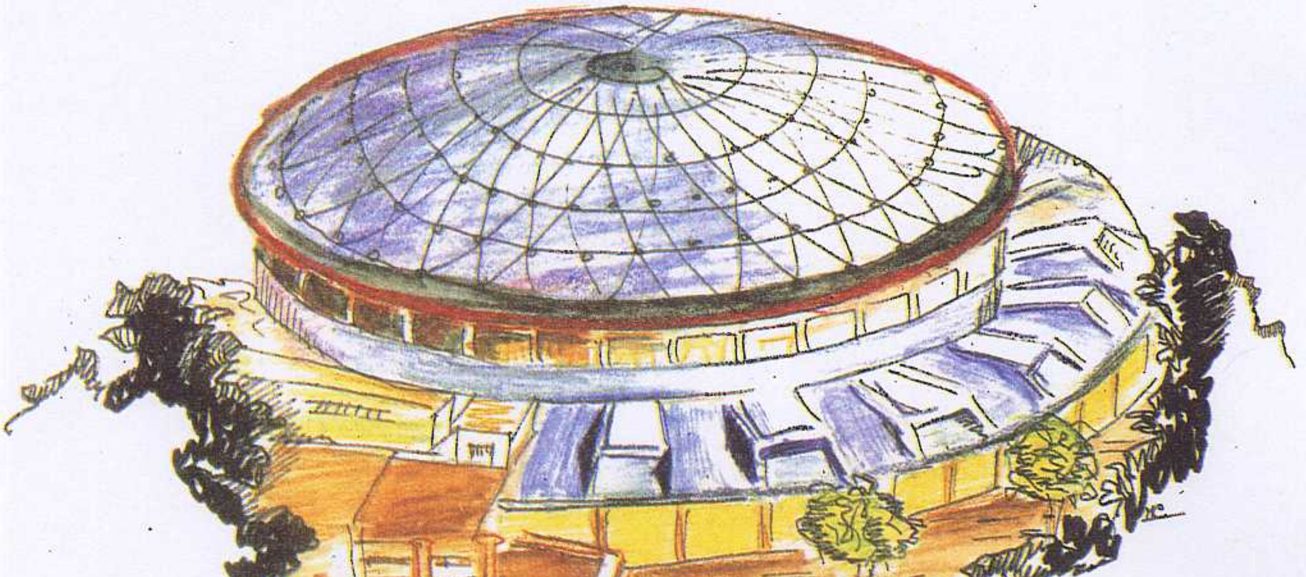
BCS SUPERCONDUCTIVITY AND THE ELECTRON-PHONON INTERACTION



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BCS SUPERCONDUCTIVITY AND THE ELECTRON–PHONON INTERACTION

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As is well known, one of the simplest formulation of the BCS–theory starts with an effective Hamiltonian:

$$H = \int d^3x \sum_{\alpha} \Psi^+_{\alpha}(\bar{x})\, H_0\, \Psi_{\alpha}(\bar{x})$$
$$+ \int d^3x_1\, d^3x_2\, d^3x_3\, d^3x_4\, \Psi^+_{\alpha}(\vec{x}_1)\, \Psi_{\beta}(\vec{x}_2)\, \Psi^+_{\alpha'}(\vec{x}_3)\, \Psi_{\beta'}(\vec{x}_4)\, V^{\alpha\beta,\alpha'\beta'}(\vec{x}_1 - \vec{x}_2, \dots) \tag{1}$$

where $V^{\alpha\beta,\alpha'\beta'}(\vec{x}_1 - \vec{x}_2, \dots)$ is an effective self–interaction of the electron field $\Psi_{\alpha}(\vec{x})$ ($\alpha = \uparrow,\downarrow$). By going to momentum space

$$\Psi_{\alpha}(\vec{x}) = \frac{1}{(V)^{1/2}} \sum_{\vec{k}} a_{\vec{k},\alpha}\, e^{i\vec{k}\vec{x}}$$

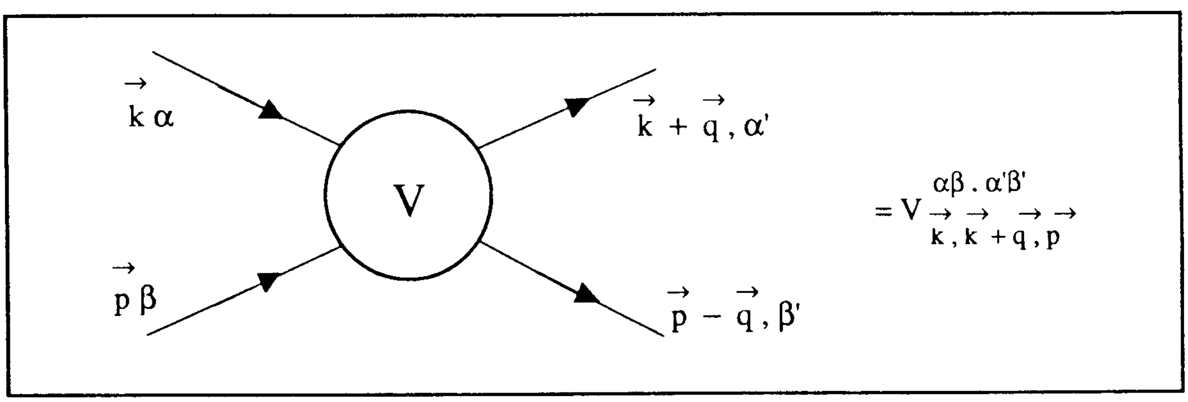
with anticommutation relations

$$\left\{a_{\vec{k}\,\alpha'},\ a^{+}_{\vec{k}'\alpha}\right\} = \delta_{\alpha\beta}\,\delta_{\vec{k},\vec{k}}$$

we can recast our Hamiltonian as

$$H = \sum_{\vec{k}} \in_{\vec{k}}\, a_{\vec{k}\,\alpha'}\, a^{+}_{\vec{n}'\alpha} \;-\; \sum_{\vec{k}\vec{p}\vec{q}\vec{q}\,'} a^{+}_{\vec{k}+\vec{q},\alpha'}\, a^{+}_{\vec{p}+\vec{q},\beta'}\, a_{\vec{p},\beta}\, a_{\vec{k},\alpha}\, V^{\alpha\beta,\alpha'\beta'}_{\vec{k},\vec{k}+\vec{q},\vec{p}} \qquad (2)$$

By considering $H - \mu N$, the only change is that the "kinetic" term the energies $\in_{\vec{k}}$ are taken from the Fermi surface, i.e $\in_{\vec{k}} \rightarrow \in_{\vec{k}} - E_F$, with $E_F = \vec{k}_F^{\,2} / 2m^*$ (m^* is the effective electron mass at the Fermi surface). The kinematics of the Potential V is decribed by the following diagram:



Superconductivity will hold if the ground state of the Hamiltonian (2) will develop a vacuum expectation value

$$A_{\vec{k}} = \langle a^{+}_{\vec{k}}\uparrow\ a^{+}_{-\vec{k}}\downarrow \rangle \neq 0. \qquad (3)$$

Due to the nature of our problem and the smallness of the energy differences from the normal degenerate vacuum, that fills all its states up to the Fermi surface, we do expect that $A_{\vec{k}}$ will be different from zero only on a thin shell of width $\simeq \Delta(o)$ – the superconductivity gap – around the Fermi surface.

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Assuming that such a configuration exists, and setting ($\vec{p} = -\vec{k}$ in the zero–momentum ground state)

$$V^{\alpha\beta,\alpha'\beta'}_{\vec{k},\vec{k}+\vec{q},\vec{p}} \simeq \delta^{\alpha\alpha'}\,\delta^{\beta\beta'}\,V_{\vec{k},\vec{k}+\vec{q}}\ , \tag{4}$$

it is a simple exercise to show that, defining the gap function

$$\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k}',\vec{k}}\,A_{\vec{k}'}, \tag{5}$$

this must obey, at T = 0, the "gap–equation"

$$\Delta_{\vec{k}} = -\sum_{\vec{k}'} V_{\vec{k},\vec{k}'}\,\frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}}\ , \tag{6}$$

where $E_{\vec{k}} = \sqrt{\epsilon^2_{\vec{k}} + \Delta^2_{\vec{k}}}$.

It is now appropriate to reexpress the kinematical variable $\vec{k}$ in a convenient way, we set

$$\vec{k} = (k_F + \frac{\epsilon}{v_F})\vec{u}\ , \tag{7}$$

where k_F is the Fermi–momentum and $v_F = \frac{k_F}{m^*}$ the Fermi–velocity. The new variable ϵ is, to first order in ϵ/v_F, equal to $\epsilon_{\vec{k}} - E_F$. Thus may write

$$A_{\vec{k}} = A\,(\epsilon,\vec{u}) = A\,(\epsilon) \tag{8}$$

where the normally valid assumption has been made that $\Delta_{\vec{k}}$ is S–wave, thus $\vec{u}$–independent. Note that, according to the discussion above, $A(\epsilon)$ is highly peaked around ϵ=0, with a width of the order $\Delta(o)$, a few degrees Kelvin. We can now make the relevant observation that, according to (5), the peaking properties of $A(\epsilon)$ are not shared by $\Delta(\epsilon)$ if the potential $V(\epsilon,\epsilon';\vec{u},\vec{u}')$ does not have a range comparable or bigger than $r \sim \frac{v_F}{\Delta(o)}$, the range of the Fourier transform of $A(\epsilon)$. This simply follows from the essential covolution nature in momentum space of Eq. (5). Thus in the generally accepted picture of the electron–phonon interaction, whose range is of the order of a few Å's, the properties of $\Delta(\epsilon)$ and $A(\epsilon)$ must be expected to differ considerably. In particular in the "gap–equation" (6) no cutting of the ϵ–

integration at the Debye–frequency is justified, due to the difference in support in ϵ between $\Delta(\epsilon)$ and $A(\epsilon)$.

Indeed let us specify the potential $V_{\vec{k},\vec{k}'}$, à la Fröhlich, i.e. let's consider

$$V_{\vec{k},\vec{k}'} = g_{\vec{k}-\vec{k}'} \frac{\omega_{\vec{k}-\vec{k}'}}{(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'})^2 - \omega^2_{\vec{k}-\vec{k}'}} \qquad (10)$$

where $g_{\vec{k}-\vec{k}'}$ is the coupling strength between an electron of initial momentum $\vec{k}$ and final momentum $\vec{k}'$ and a phonon of momentum $\vec{k}-\vec{k}'$, and energy (v_s is the velocity of sound)

$$\omega_{\vec{k}-\vec{k}'} \simeq v_s \left|\vec{k}-\vec{k}'\right|. \qquad (11)$$

$g^2_{\vec{q}}$ is a slowly varying function of $\omega_{\vec{q}}$ and can be well approximated by a constant $\bar{g}^2$. In the new variables we may cast the potential (10) in the form

$$V(\epsilon\ \epsilon';\ \vec{u}\ \vec{u}') = \frac{\bar{g}^2}{V} \frac{\omega_{\vec{u},\vec{u}'}}{(\epsilon-\epsilon')^2 - \omega^2_{\vec{u},\vec{u}'}} \qquad (12)$$

where

$$\omega_{\vec{u},\vec{u}'} \cong \sqrt{2}\,\omega_D \left(1 - \cos\theta_{\vec{u},\vec{u}'}\right)^{1/2} \leq \omega_D, \qquad (13)$$

where we have used the fact that $k_F \gg \frac{\epsilon}{v_F}, \frac{\epsilon'}{v_F}$, and set the Debye frequency $\omega_D \simeq v_s\, k_F$. Changing variables and using (12) we can rewrite the "gap–equation" (6) as:

$$\Delta(\epsilon) = -\lambda \int_{-E_F}^{E_F} d\epsilon' \frac{w(\epsilon-\epsilon')\Delta(\epsilon')}{\sqrt{\epsilon'^2 + \Delta(\epsilon')^2}} \qquad (14)$$

where $\lambda = \frac{k_F^2}{2\omega_D v_F} \frac{\bar{g}^2}{4\pi^2}$, and

$$w(x) = -1 + \frac{x}{2\omega_D} \ln \left| \frac{1 + \frac{x}{\omega_D}}{1 - \frac{x}{\omega_D}} \right| . \tag{15}$$

Note that we have not cut–off the ϵ integration at ω_D,where the potential w(x) is essentially attractive, but rather at the more reasonable value $E_F >> \omega_D$, a range which includes a great deal of repulsion (for $x > \omega_D$). We recall that the "BCS approximation" consists in setting $w(\epsilon - \epsilon') \simeq -1$ for $|\epsilon - \epsilon'| < \omega_D$ and $w(\epsilon - \epsilon')=0$ for $|\epsilon - \epsilon'| > \omega_D$, and note that it would be a perfectly reasonable Ansatz if, instead of $\Delta(\epsilon)$, the wave–function $A(\epsilon)$ appeared in the gap–equation. But, as stressed above, this is not what is implied by Eq. (5). Indeed going to the ϵ–variable, and using the strong peaking of $A(\epsilon)$ (recall $\Delta(o) \ll \omega_D$), one easily obtains

$$\Delta(\epsilon) \simeq -\Delta(o)\, w(\epsilon), \tag{16}$$

where $\Delta(o)$ is the value of the gap in the vicinity of the Fermi–surface. Assuming $\Delta(o) \neq 0$ and substituting (16) in Eq. (14) the "gap–equation" becomes

$$w(\epsilon) = -\lambda \int_{-E_F}^{E_F} d\epsilon' \frac{w(\epsilon - \epsilon')\, w(\epsilon')}{\sqrt{\epsilon'^2 + \Delta(o)^2\, w(\epsilon')^2}} , \tag{17}$$

which implies the following equations

$$1 = +\lambda \int_{-E_F}^{E_F} d\epsilon' \frac{w(\epsilon')^2}{\sqrt{\epsilon'^2 + \Delta(o)^2\, w(\epsilon')^2}} , \tag{17'}$$

$$1 = -\lambda \int_{-E_F}^{E_F} d\epsilon' \frac{w(\epsilon')}{\sqrt{\epsilon'^2 + \Delta(o)^2\, w(\epsilon')^2}} , \tag{17''}$$

for $\epsilon = 0$ and $\epsilon \to \infty$ respectively. By taking the difference one gets

$$O = \int_{-E_F}^{E_F} d\epsilon \; \frac{w(\epsilon)^2 + w(\epsilon)}{\sqrt{\epsilon^2 + \Delta(o)^2 \, w(\epsilon)^2}} \tag{18}$$

A simple calculation shows the integral to have the non–zero value $1 - \frac{1}{3}\left(\frac{\omega_D}{E_F}\right)^2 + O\left[\left(\frac{\omega_D}{E_F}\right)^4\right]$, demonstrating the inconsistency between a non vanishing $\Delta(o)$ and the effective electron–electron potential being dominated by a short–range electron–phonon interaction. Naturally the inconsistency we have thus exposed is a rather weak consequence of the much stronger constraints (17), that the electron–phonon potential (15) is in no way capable to fulfill.

We must therefore conclude that the inclusion in the BCS gap equation of the repulsive part of the short–range electron–phonon interaction is sufficient to prevent the existence of any non–trivial solution, contrary to what happens when the repulsive part is arbitrarily cut–off.