

The Cooper pair problem in an external periodic potential

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Recibido el 9 de julio de 1999; aceptado el 18 de febrero de 2000

We propose and approximately solve the problem of an existing Cooper pair system under the presence of an external periodic potential. Expressions for the energy gap and the critical superconducting temperature for a superconductor under these conditions are calculated, both quantities being affected by the external potential, although their ratio remains unchanged.

Keywords: BCS model; energy gap; weak coupling

Se propone y resuelve aproximadamente el problema de los pares de Cooper ante la presencia de un potencial periódico externo. Se obtienen expresiones explícitas para la energía de ligadura del par de Cooper, así como de la brecha y la temperatura crítica superconductor bajo las condiciones propuestas. Se encuentra que los parámetros mencionados se ven afectados por la presencia del potencial externo, pero el cociente entre la brecha superconductor y la temperatura crítica permanece inalterado.

Descriptores: Modelo BCS; brecha superconductor; acoplamiento débil

PACS: 74.20.Fg

1. Introduction

The central ingredient in the Bardeen, Cooper and Schrieffer (BCS) theory of superconductivity is the existence of so-called Cooper pairs [1]. Specifically, the ground state ($T=0$ K) of an electron gas becomes unstable under an attractive interaction between electron pairs. Since the Coulomb interaction between electrons is always repulsive, another mechanism is needed in order to have a net effective attractive interaction. In the traditional BCS theory, this attractive interaction between electrons is an electron-phonon coupling. In effect, then, the pair of electrons are attracted to each other via a lattice deformation. This attraction must overwhelm the Coulomb repulsion so that Cooper pairs might be formed.

The idea followed here is not to find the mechanism by which electrons bind into pairs, but rather to consider introducing a periodic external potential which affects the existing electron pair.

A periodic external potential can arise as follows. A superconducting thin film deposited on a ionic substrate where a square lattice of alternating positive and negative ions will produce an external periodic potential affecting the vicinity of the superconductor interface. This potential will penetrate into the superconductor by just a few layers, but we may idealize the problem by assuming an infinite superconducting system in a periodic external potential.

Another approach is to consider superlattices of superconducting and normal metals in alternating layers. If the thickness of the normal metal is small enough compared to that of the superconductor layer, we can consider the whole system as the superconductor embedded into a quasi-one-dimensional periodic potential, such as has been treated by other authors [2].

Finally, one interesting system which has a superlattice-like structure is the superconducting ceramic $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. In this case, Cu-O planes are sandwiched between Ba-O and

Y planes stacked along the c direction of the unit cell [3]. To date, it is generally thought that the superconducting properties of this material are dominated by the Cu-O planes [3, 4]. We propose that our model may be an idealized approach to this system, in which the superconductivity lies in the Cu-O planes separated by non-superconducting Ba-O and Y layers. Here the periodic potential is provided by the atoms forming the non-superconducting spacers, but together forming the whole system.

In successive sections we adopt the BCS problem of superconductivity in the traditional approach, namely by assuming a constant attractive potential between pairs of electrons in reciprocal space, but also adding an external potential to the pairs.

2. The binding energy of the Cooper pair

A simple way of modelling the periodic external potential $V(\mathbf{r})$ acting on the Cooper pair is by writing, for an electron at \mathbf{r} ,

$$V(\mathbf{r}) = A \cos(\mathbf{G} \cdot \mathbf{r}),$$

where \mathbf{G} is the wavevector representing the spatial periodicity of the potential. If \mathbf{r}_1 and \mathbf{r}_2 are the positions of the two electrons in the pair, the potential energy of the pair is then

$$\begin{aligned} V_{\text{ext}} &= A \cos(\mathbf{G} \cdot \mathbf{r}_1) + A \cos(\mathbf{G} \cdot \mathbf{r}_2) \\ &= 2A \cos \left[\mathbf{G} \cdot \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right) \right] \cos \left[\mathbf{G} \cdot \left(\frac{\mathbf{r}_1 - \mathbf{r}_2}{2} \right) \right]. \end{aligned}$$

If we now consider states with center-of-gravity of the pair at rest [5], the quantity $(\mathbf{r}_1 + \mathbf{r}_2)/2$ is constant and the potential depends solely on the relative coordinates of the pair.

Consequently, we take the following idealized potential energy of the pair due to the external periodic potential

$$V_{\text{ext}} = -V_1 \cos(\mathbf{G} \cdot \mathbf{r}), \tag{1}$$

where we redefined the amplitude V_1 of the interaction as a positive parameter, the new wavevector \mathbf{G} has taken the place of $\mathbf{G}/2$, and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is the relative position of the electrons in the pair. From Eq. (1) the interaction between electrons of the pair will be attractive or repulsive depending on their relative positions.

The usual procedure to solve the Schrödinger-like equation in momentum space associated with the Cooper pair can be followed. In reciprocal space [6] one has for the binding energy eigenvalue E

$$\frac{\hbar^2 k^2}{m} g(\mathbf{k}) + \sum_{\mathbf{k}'} g(\mathbf{k}') V_{\mathbf{k}\mathbf{k}'} = (E + 2E_F) g(\mathbf{k}), \tag{2}$$

where E_F is the Fermi energy associated with the background electrons, and $g(\mathbf{k})$ is the probability amplitude for finding one electron in state \mathbf{k} and the other in state $-\mathbf{k}$, while $V_{\mathbf{k}\mathbf{k}'}$ is the interaction matrix element between these electrons. As usual in the BCS theory, $g(\mathbf{k})$ is zero out of the interval in energy from E_F to $E_F + \hbar\omega_D$, where $\hbar\omega_D$ is the Debye energy. Specifically,

$$V_{\mathbf{k}\mathbf{k}'} = \frac{1}{L^3} \int V(\mathbf{r}) e^{-i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} d\mathbf{r}, \tag{3}$$

where $V(\mathbf{r})$ is the total interaction between electrons in the pair and L^3 is the system volume. Rewriting Eq. (1) in complex form, it is not difficult to show that Eq. (3) becomes

$$V_{\mathbf{k}\mathbf{k}'} = -V_0 - \frac{V_1}{2L^3} [\delta(\mathbf{k}' - \mathbf{k} + \mathbf{G}) + \delta(\mathbf{k}' - \mathbf{k} - \mathbf{G})], \tag{4}$$

for

$$E_F < \frac{\hbar^2 k^2}{2m} < E_F + \hbar\omega_D,$$

and

$$V_{\mathbf{k}\mathbf{k}'} = 0 \quad \text{otherwise.}$$

Here, $-V_0$ is the usual BCS model attractive interaction which produces pairing of the electrons. The second term in Eq. (4) arises from the external potential Eq. (1). In Eq. (4) we assume that the external potential is nonzero only in energy states within the Debye energy $\hbar\omega_D$ above the Fermi energy E_F , since we consider only on an existing pair already bound by the intrinsic constant attractive pair potential term $-V_0$.

The problem is now to solve Eq. (2) given the interaction model Eq. (4). To solve this problem exactly is a difficult task, but use an approximate procedure in order to obtain an explicit form for the pair binding energy under the periodic external potential added.

Inserting Eq. (4) into Eq. (2) and arranging terms one gets

$$V_0 \sum_{\mathbf{k}'} g(\mathbf{k}') + \frac{V_1}{2L^3} \sum_{\mathbf{k}'} g(\mathbf{k}') [\delta(\mathbf{k}' - \mathbf{k} + \mathbf{G}) + \delta(\mathbf{k}' - \mathbf{k} - \mathbf{G})] = \left(\frac{\hbar^2 k^2}{m} - E - 2E_F \right) g(\mathbf{k}). \tag{5}$$

Replacing sums over \mathbf{k}' by integrals in the form [7]

$$L^{-3} \sum_{\mathbf{k}'} \rightarrow \frac{1}{(2\pi)^3} \int d\mathbf{k}',$$

and noting that

$$\frac{V_0}{(2\pi)^3} \int g(\mathbf{k}') d\mathbf{k}' = C \tag{6}$$

is a constant, we can then write:

$$g(\mathbf{k}) = \frac{CL^3}{2\varepsilon(\mathbf{k}) - E - 2E_F} + \frac{V_1}{2} \frac{(2\pi)^{-3} \int g(\mathbf{k}') [\delta(\mathbf{k}' - \mathbf{k} + \mathbf{G}) + \delta(\mathbf{k}' - \mathbf{k} - \mathbf{G})] d\mathbf{k}'}{2\varepsilon(\mathbf{k}) - E - 2E_F}, \tag{7}$$

where $\varepsilon(\mathbf{k}) \equiv \hbar^2 k^2 / 2m$. Evaluating the integral in Eq. (7) and using Eq. (6), we finally obtain

$$C = \frac{CL^3 V_0}{(2\pi)^3} \int \frac{d\mathbf{k}'}{2\varepsilon(\mathbf{k}') - E - 2E_F} + \frac{V_0 V_1}{2(2\pi)^6} \int \frac{[g(\mathbf{k}' - \mathbf{G}) + g(\mathbf{k}' + \mathbf{G})]}{2\varepsilon(\mathbf{k}') - E - 2E_F} d\mathbf{k}'. \tag{8}$$

Note from Eq. (8) that if the external potential amplitude V_1 is zero, one recovers the expression for the familiar Cooper pair binding energy equation.

To solve Eq. (8), we need to know an expression for $g(\mathbf{k})$, as a first approximation suppose the amplitude V_1 small enough such that from Eq. (7) $g(\mathbf{k})$ can be taken as the first

term of the right side, namely,

$$g(\mathbf{k}) \simeq \frac{CL^3}{2\varepsilon(\mathbf{k}) - E - 2E_F}. \tag{9}$$

Using this to evaluate $g(\mathbf{k}' - \mathbf{G})$ and $g(\mathbf{k}' + \mathbf{G})$ which are

then inserted into Eq. (8) leads to the self-consistent equation:

$$1 = \frac{L^3 V_0}{(2\pi)^3} \int \frac{d\mathbf{k}}{2\varepsilon(\mathbf{k}) - E - 2E_F} + \frac{L^3 V_0 V_1}{2(2\pi)^6} \int \left[\frac{1}{2\varepsilon(\mathbf{k} - \mathbf{G}) - E - 2E_F} + \frac{1}{2\varepsilon(\mathbf{k} + \mathbf{G}) - E - 2E_F} \right] \frac{d\mathbf{k}}{2\varepsilon(\mathbf{k}) - E - 2E_F}. \quad (10)$$

In principle, Eq. (10) might be solved for the binding pair energy E , given specific values of V_0 , V_1 , E_F , and \mathbf{G} . However, we make further simplifications in order to seek an explicit solution for E . The following supposition might be an approximation to a superlattice (see introduction) where the vector \mathbf{G} is perpendicular to the layers and the movement of the electrons is mainly confined to run parallel to the superconducting layers. As a first approximation to this situation we can suppose that vectors \mathbf{k} and \mathbf{G} are mutually perpendicular.

The explicit form of $\varepsilon(\mathbf{k} - \mathbf{G})$ and $\varepsilon(\mathbf{k} + \mathbf{G})$ are

$$\varepsilon(\mathbf{k} \mp \mathbf{G}) = \frac{\hbar^2}{2m} (\mathbf{k} \mp \mathbf{G})^2 = \frac{\hbar^2}{2m} (k^2 \mp 2\mathbf{k} \cdot \mathbf{G} + G^2),$$

and assuming for simplicity that $\mathbf{k} \cdot \mathbf{G} = 0$, we then have that

$$\varepsilon(\mathbf{k} - \mathbf{G}) = \varepsilon(\mathbf{k} + \mathbf{G}) = \varepsilon(\mathbf{k}) + \frac{\hbar^2 G^2}{2m}. \quad (11)$$

To further simplify solving Eq. (10) one can integrate over energy ε instead of over wavevector \mathbf{k} by introducing the density of electronic states $N(\varepsilon)$ for one spin in the form

$$d\mathbf{k} = \frac{(2\pi)^3}{L^3} N(\varepsilon) d\varepsilon, \quad (12)$$

noting that since $E_F < \varepsilon < E_F + \hbar\omega_D$, $N(\varepsilon)$ can be taken as a constant equal to $N(E_F)$ provided that $N(\varepsilon)$ does not vary appreciably within this small interval of energy because $\hbar\omega_D \ll E_F$. Using Eq. (11), Eq. (10) reduces to

$$1 = V_0 N(E_F) \int_{E_F}^{E_F + \hbar\omega_D} \frac{d\varepsilon}{2\varepsilon - E - 2E_F} + \frac{V_0 V_1 N(E_F)}{(2\pi)^3} \int_{E_F}^{E_F + \hbar\omega_D} \frac{d\varepsilon}{(2\varepsilon - E - 2E_F)(2\varepsilon - E - 2E_F + \hbar^2 G^2/m)}, \quad (13)$$

which can be integrated exactly. After some algebra, one obtains

$$\left(\frac{E - 2\hbar\omega_D}{E} \right)^{1+\alpha} \left(\frac{E - \hbar^2 G^2/m}{E - 2\hbar\omega_D - \hbar^2 G^2/m} \right)^\alpha = e^{\frac{2}{\lambda}}, \quad (14)$$

where $\lambda \equiv V_0 N(E_F)$ is the BCS superconducting coupling constant and α is defined as

$$\alpha \equiv \frac{V_1}{(2\pi)^3} \frac{m}{\hbar^2 G^2}. \quad (15)$$

Note that α contains essential information about the external potential such as the amplitude V_1 and the spatial periodicity G .

To make even further simplifications in Eq. (14), let us estimate the order of magnitude of the quantity $\hbar^2 G^2/m$. Since $G \sim 2\pi/d$, where d represents the spatial periodicity of the external potential, taking $d \sim (1-10) \text{ \AA}$ gives $G \sim 2\pi(1-10^{-1}) \text{ \AA}^{-1}$, and finally $\hbar^2 G^2/m \sim (300-3) \text{ eV}$. On the other hand, in elemental superconductors $\hbar\omega_D \sim (6-36) \times 10^{-3} \text{ eV}$ [8]. Thus, in Eq. (14) the second factor of the left hand side can be approximated by unity since $\hbar^2 G^2/m \gg 2\hbar\omega_D$. Hence the binding energy of the pair becomes

$$E \simeq \frac{2\hbar\omega_D}{1 - e^{2/\lambda(1+\alpha)}},$$

this reduces to the familiar solutions when $V_1 = 0$, which implies $\alpha = 0$. In the limit of weak coupling, interaction, taken as when $V_0 N(E_F)(1 + \alpha) \ll 1$, this finally leads to:

$$E = -2\hbar\omega_D e^{-\frac{2}{\lambda(1+\alpha)}}. \quad (16)$$

From Eq. (16) the energy E being negative corresponds to a *bound* state and is similar to that of the familiar Cooper pair problem save for the additional factor $(1 + \alpha)$ multiplying the coupling constant $V_0 N(E_F)$. We have then arrived at the following important result: the binding energy of the pair of Cooper electrons is *increased* or *decreased* according to whether V_1 is positive or negative respectively, by the presence of an periodic external potential.

3. The energy gap and the critical superconducting transition temperature

Two important parameters that characterize the BCS superconducting state are the energy gap Δ (which is related to the energy necessary to break the Cooper pair) and the critical temperature T_C below which the normal state becomes superconducting.

To determine the energy gap at $T = 0 \text{ K}$, we start from the self-consistent gap equation [9] given by:

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} V_{\mathbf{k}\mathbf{k}'}, \quad (17)$$

where $V_{\mathbf{k}\mathbf{k}'}$ is given by Eq. (4) and $E_{\mathbf{k}'} \equiv \sqrt{\Delta_{\mathbf{k}'}^2 + \xi_{\mathbf{k}'}^2}$, with $\xi_{\mathbf{k}'} \equiv \varepsilon(\mathbf{k}') - E_F$. Converting Eq. (17) to integral form gives,

$$\Delta(\mathbf{k}) = \frac{V_0}{2(2\pi)^3} \int \frac{\Delta(\mathbf{k}')}{E(\mathbf{k}')} d\mathbf{k}' + \frac{V_1}{4(2\pi)^3} \left[\frac{\Delta(\mathbf{k} - \mathbf{G})}{E(\mathbf{k} - \mathbf{G})} + \frac{\Delta(\mathbf{k} + \mathbf{G})}{E(\mathbf{k} + \mathbf{G})} \right], \tag{18}$$

where the integral on the right hand side of Eq. (18) is independent of the wave vector and thus a constant, say Δ_0 , given by

$$\Delta_0 = \frac{V_0}{2(2\pi)^3} \int \frac{\Delta(\mathbf{k}')}{E(\mathbf{k}')} d\mathbf{k}'. \tag{19}$$

Substituting $\Delta(\mathbf{k}')$ from Eq. (18) into Eq. (19) leads to

$$\Delta_0 = \frac{V_0}{2(2\pi)^3} \left\{ \Delta_0 \int \frac{d\mathbf{k}'}{E(\mathbf{k}')} + \frac{V_1}{4(2\pi)^3} \int \left[\frac{\Delta(\mathbf{k}' - \mathbf{G})}{E(\mathbf{k}')E(\mathbf{k}' - \mathbf{G})} + \frac{\Delta(\mathbf{k}' + \mathbf{G})}{E(\mathbf{k}')E(\mathbf{k}' + \mathbf{G})} \right] d\mathbf{k}' \right\}. \tag{20}$$

Assuming as a first approximation that the energy gap is independent of the wave vector and given by Δ_0 , Eq. (20) becomes

$$1 = \frac{V_0}{2(2\pi)^3} \left\{ \int \frac{d\mathbf{k}'}{E(\mathbf{k}')} + \frac{V_1}{4(2\pi)^3} \int \left[\frac{1}{E(\mathbf{k}')E(\mathbf{k}' - \mathbf{G})} + \frac{1}{E(\mathbf{k}')E(\mathbf{k}' + \mathbf{G})} \right] d\mathbf{k}' \right\}. \tag{21}$$

As before, assuming \mathbf{G} perpendicular to wave vector \mathbf{k}' , and integrating over energy ξ instead of over wavevectors, this reduces to:

$$1 = \frac{V_0 N(E_F)}{2} \left\{ \int \frac{d\xi}{\sqrt{\Delta_0^2 + \xi^2}} + \frac{V_1}{2(2\pi)^3} \int \frac{d\xi}{\sqrt{\Delta_0^2 + \xi^2} \sqrt{\Delta_0^2 + (\xi + \hbar^2 G^2/2m)^2}} \right\}. \tag{22}$$

To further simplify evaluation of Eq. (22) suppose that $\hbar^2 G^2/2m \gg \Delta_0$ or ξ , which is reasonable since Δ_0 is of the order of a few meV [10] and ξ varies by at most $\hbar\omega_D$. Under these conditions Eq. (22) simplifies to

$$\begin{aligned} 1 &\simeq \frac{V_0 N(E_F)}{2} (1 + \alpha) \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\xi}{\sqrt{\Delta_0^2 + \xi^2}} \\ &= V_0 N(E_F) (1 + \alpha) \sinh^{-1} \left(\frac{\hbar\omega_D}{\Delta_0} \right), \end{aligned} \tag{23}$$

where α is again given by Eq. (15). In the weak coupling limit Eq. (23) finally leads to

$$\Delta_0 = 2\hbar\omega_D e^{-\frac{1}{V_0 N(E_F)(1+\alpha)}}. \tag{24}$$

On the other hand, to find a expression for T_C , we need the temperature-dependent self consistent gap equation [11] given by

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} V_{\mathbf{k}\mathbf{k}'} \tanh \left(\frac{\beta E_{\mathbf{k}'}}{2} \right), \tag{25}$$

where $\beta = 1/k_B T$, k_B the Boltzmann constant, and T the absolute temperature. Starting from Eq. (25) and using the same procedures as those to find Δ_0 , it is not difficult to find an expression for T_C as a solution of $\Delta(T_C) = 0$, which is

$$kT_C = 1.13\hbar\omega_D e^{-\frac{1}{V_0 N(E_F)(1+\alpha)}}. \tag{26}$$

Note that Eqs. (24) and (26) are similar to the familiar BCS expressions save for the coupling constant λ becoming $V_0 N(E_F)(1 + \alpha)$. Here we see that both the energy gap at

$T = 0$ K (Δ_0) and the critical temperature T_C are affected by the presence of the periodic external potential through the parameter α . However, although both Δ_0 and T_C are modified by the external potential, their ratio is unchanged, at least in the limit of weak coupling.

4. Discussion

The usual intuitive picture of the formation of the Cooper pair is that one electron, travelling through the background of positive ions, pulls positive ions of the lattice forming momentarily an excess of positive charge in some spatial region of the lattice. This excess of positive charge, due to the deformation of the lattice, is seen by the second electron which is attracted to that region. The whole event is that the two electrons are attracted together via the deformation of the lattice.

The picture for our model may be viewed as follows. Imagine that the external periodic potential produces in the lattice fringes of attractive and repulsive regions for the electrons, modulated by the wavevector of the external potential. In some event, an attractive fringe may spatially coincide with the deformation of the lattice produced by the first electron, reinforcing in this way the attractive action for the second electron. In this case, the magnitude of the binding energy of the Cooper pair will increase (see last paragraph of Sect. 2). The opposite situation is expected when the accumulation of positive ions produced by the first electron lies in a repulsive fringe of the external potential.

Obviously, this picture is a very crude view of a more complicated phenomena, in which some kind of coupling between the periodicity of the external potential and some characteristic length (related to a spatial extent of the Cooper pair) could exist.

5. Conclusion

We have studied the problem of the binding energy of a Cooper pair in the presence of a periodic external potential. We also studied the effect of the periodic external potential

on the zero temperature energy gap and the critical temperature of the system within the standard BCS formalism. Assumptions were made to analytically solve the resulting self-consistent equations. Both parameters, energy gap at $T = 0\text{K}$ and T_C , are modified by the presence of the periodic external potential, but their ratio remains unchanged.

Acknowledgments

I want to thank M. de Llano for fruitful discussions which improved the present work.

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