Model for p- and d-wave superconductivity in heavy-fermion systems

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The possibility of p- and d-wave superconductivity with the two electron constituents of the Cooper pair in a relative angular momentum $l=1$ or 2 and $m=0$ state with respect to their axis of relative motion is studied. In order for the corresponding wave function to be localized within the binding potential, the effective masses of the electrons have to be high. These considerations apply to heavy-fermion systems such as UPt_3 and UBe_{13}.

Recent experiments[1,2] indicate a new type of electron pairing in the superconducting phase of heavy-fermion systems, such as UBe_{13} and UPt_3, associated with a relative angular momentum of the electrons forming the Cooper pair of $l\neq 0$. While this possibility has been considered ever since the Bardeen-Cooper-Schrieffer (BCS) theory was introduced,[3] in this context it has been proposed by Varma[4] and Anderson[5] (while Tachiki and Maekawa[6] and consequently Razafimandimby, Fulde, and Keller[7] suggested applying conventional s pairing of the electrons in the $l=0$ configuration to explain the experimental findings). In the following I shall argue that, depending on the effective electron mass, which must at least be of the order of a few hundred vacuum electron masses, a p and d state yields a binding and the appearance of a superconducting energy gap similar to s-wave pairing.

The widely accepted heuristic notion of a Cooper pair[8] is that of two electrons in a relative s state[9,10] formed by a linear combination of electron motions away and towards one another, with spins antiparallel (see Fig. 1). This oscillation is made possible by a dynamic equilibrium between Coulomb repulsion and attractive phonon interaction, mediated by ionic vibrations polarizing the lattice.[11] In what follows this potential problem is studied in greater detail, assuming a model "potential tube" behind each electron (see Fig. 2). Since this potential corresponds to a highly distorted spherical potential, it will not be invariant under the rotation group SO(3), but rather under D_∞, and the bound-state solutions will be very difficult to enumerate explicitly. If one approximates them by solutions of spherical symmetric potentials (which is a quite naive and rough procedure), only the $m=0$ states with wave functions concentrated along the axis of electron movement will be dynamically allowed, since otherwise the electron wave function would not be appreciably within the highly assymmetric pairing potential.

In what follows a qualitative model is applied to construct the pairing potential. Following Weisskopf,[9] this potential is then inserted into the Schrödinger equation and applied to the calculation of the pair wave function and the energy spectrum. The binding energy is then identified with the superconducting energy gap, which assumes the well-known BCS expression. It turns out that $l=1$, $m=0$ and $l=2$, $m=0$ states (with the m number measured parallel to the potential tube) acquire energy gaps of the same type, only differing by the density of states at the Fermi surface. Whether these $l=1$ and 2 states exist depends on the length of the potential tube compared to the mean distance of the electrons in this state: Heuristically speaking, if "most" of the electron pair wave function is within the potential tube, both electrons feel this binding potential. This is also the reason why the $m\neq 0$ states do not contribute. The mobility of the electrons and, in turn, the extension of their wave functions depend on the effective masses.

In the following I shall give a brief sketch of Weisskopf's approach[9] and consider a cubic lattice of positive ions with lattice distance a, filled with a degenerate gas of free atoms, one per ion. In such a lattice, electrons at the Fermi surface travel with velocities of approximately $v\sim p_F/m\sim 1/ma$, where p_F is the Fermi momentum, m the electron mass, and Planck's constant h has been set to one. The electrons spend a time $\tau\sim a/v$ within a distance a from a given ion, and thereby transfer a momentum $p\sim V\tau/a$ to the ion, where V is the Coulomb potential, $V=e^2/a\sim 1/ma^2$. If the ion is assumed to be coupled linearly only to its nearest neighbor, we obtain from oscillator dynamics that its displacement due to momentum transfer is given by $\delta\sim p/M\omega_D$, where M is the ion mass and ω_D is the Debye frequency entering the oscillator potential $M\omega_D^2\delta^2/2$, which can be identified with the average ionic Coulomb potential V, yielding $\omega_D\sim V/\beta$, where $\beta:=(M/m)^{1/2}\sim 100$ for usual values of M and m. With this, the average ionic displacement for an electron passing the ion is $\delta\sim a/\beta$. Assuming an average relaxation time of the order of ω_D^{-1}, the poten-

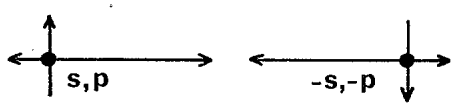

FIG. 1. Two correlated electrons forming a Cooper pair in an s state.

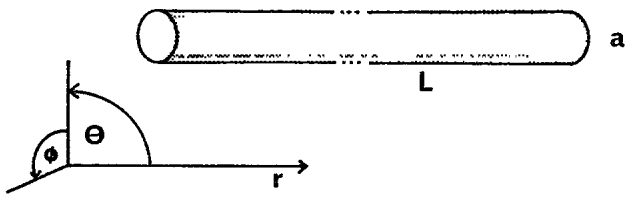

FIG. 2. The model potential tube behind each electron. It is a cylinder with a diameter of one lattice distance a and with a length L of the order of a few hundred lattice distances.

tial will extend over a distance

$$L = v\omega_D^{-1} = a\beta \quad (1)$$

behind the electron. From these qualitative considerations it follows that the potential tube formed by an electron passing through the lattice is a kind of narrow tail, approximately 100 lattice spacings long, with a diameter of not more than a single lattice distance, produced by ions less than $\frac{1}{100}$ of a lattice distance displaced. Since a displacement δ changes the ordinary potential $V = e^2/a$ of an ion by $U \sim e^2\delta/a^2 \sim e^2/L$, it is possible to formulate a mutual binding potential for the electrons in a Cooper pair by

$$U(r) = -\frac{e^2}{L}\delta_{m0}\theta(L-r)\theta(L-d[l]) \ , \quad (2)$$

where the function $d[l]$ indicates the average electron distance. In a naive model, $d[l]$ is approximated by values from a spherical symmetric Coulomb potential $d[l] \sim a[3n^2 - l(l+1)]$, where n stands for the principal quantum number.

The potential $U(r)$ in (2) is constant up to the distance L, where it is cut to zero. The second Heavyside function refers to the total angular momentum l. Assuming that the wave function of the two electrons in the s state ($n=1$ and $l=m=0$) is concentrated at an average distance of less than or equal to a, their distance in an $l \neq 0$ state can be estimated to be of the order of[12] $d[l]$. In order for the electrons to feel the attractive potential, the wave function has to appreciably overlap the potential, yielding the requirement that $L \geq d[l]$. The δ_{m0} function is necessary since the potential is highly asymmetric, such that only states with $m=0$ with respect to the potential axis are assumed to contribute for the same overlap reasoning as above. The eigenstates and the associated energy eigenvalues can be obtained by a factorization of the radial part of the pair wave function from the angular-dependent part:[13,14]

$$\psi_{p,l,m}(r,\theta,\phi) = n_l j_l(pr)\, Y_{lm}(\theta,\phi) \ , \quad (3)$$

where n_l is a normalization factor for a large sphere of radius R. The radial part is given by

$$j_l(z) = (-1)^l z^l \left(\frac{d}{z\,dz}\right)^l \frac{\sin z}{z} \ . \quad (4)$$

With the functions Y_{lm} normalized, the three-dimensional problem can be reduced to a one-dimensional problem if the radial wave function is multiplied by r. Hence, the following wave function can be defined:

$$\Psi(p) := \int r\psi_{p,l,m}\, d\theta\, d\phi = n_l r j_l(pr) \ , \quad (5)$$

and the superposition of states

$$\Psi(r) = \sum_{p'} \alpha(p')\Psi(p') \ . \quad (6)$$

Equations (4) and (5) yield the wave functions of the $l=0, 1$, and 2 states:

$$\Psi_0(p) = \frac{2}{R}\sin(pr) \ , \quad (7a)$$

$$\Psi_1(p) = \frac{2}{R}\left(\frac{\sin(pr)}{pr} - \cos(pr)\right) \ , \quad (7b)$$

$$\Psi_2(p) = \frac{2}{R}\left[\left(\frac{3}{(pr)^2} - 1\right)\sin(pr) - \frac{3\cos(pr)}{pr}\right] \ . \quad (7c)$$

The Schrödinger equation of the pair function can then be written as

$$\left(\frac{p^2}{m} + U\right)\Psi = E\Psi \ , \quad (8)$$

with the binding potential $U(r)$ from (2). This one-dimensional problem has solutions (6) with coefficients

$$\alpha(\epsilon_p) = (\epsilon_p + \Delta)^{-1} \ , \quad (9)$$

where the energy variable $\epsilon_p = (p^2 - p_F^2)/m$ instead of p has been introduced as argument of the weight function α. In this energy scale, the Fermi energy $\epsilon_F = 0$ and the eigenvalue E will be the negative binding energy of the pair, $E = -\Delta$. The gap function Δ is interpreted here as the binding energy, and turns out to be analogous to the BCS expression

$$\Delta = \omega_D \exp\left(-\frac{1}{uN[l]}\right) \ , \quad (10)$$

where $u = e^2/L$ and $N[l]$ is the density of l-pairing states at the Fermi surface. Thus, in this approximation we find the same type of gap dependence for arbitrary l (we have shown $l=1,2$). Whether $l \neq 0$ pairing is possible depends very much on the length of the potential tube compared to the mobility of the electrons forming that pair. The average momentum spread Δp of a bound state is connected to its binding energy Δ by the relation[8] $\Delta p = m\Delta/p_F$. An approximate measure for the extension of the wave function can be defined by $\rho \sim 1/\Delta p \sim p_F^2 a/m\Delta$. This compares to the length of the potential tube: For usual s-wave superconductors, the ratio $Q := \rho/L \sim p_F^2/\Delta(mM)^{1/2}$ is small enough for the s-wave function to be within the potential tube, but too large for the p-wave function to be included. For this kind of potential[14] the relative expansion of the states with $l=0$ and 1 is approximately given by $d[0]:d[1] \sim 1:10$. With the requirement that the wave function is well confined within the potential tube, $Q(m^*, l=1) \sim Q(m, l=0)$ [where $Q(m^*, l=1) \sim 10p/L$], in order for the system to be a p-wave superconductor it should contain electrons with effective masses m^* of at least equal to or greater than $100m$. Similar considerations apply for d pairing, since in the $n=3$, $l=1$ configuration, $m^* \sim 600m$ and in the $n=3$, $l=2$ configuration, $m^* \sim 400m$.

In conclusion, it should be noted that the following inputs have been made: (i) strongly simplified lattice dynamics yielding a potential tube behind the electrons, and (ii) spherical symmetric pair wave functions with distance behavior as for of the Coulomb potential. These are rather rough approximations which can be considered only as first estimates of the dynamics involved. However, the results obtained agree well with values observed in heavy-fermion systems, where $m^* = O((10^2-10^3)m)$ and may serve as an additional indication for $l \neq 0$ superconductivity. Future experiments may confirm this evidence further.

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