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LETTER TO THE EDITOR

Two phase transitions in (s + id)-wave Bardeen–Cooper–Schrieffer superconductivity

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Abstract. We establish universal behaviour in the temperature dependencies of some observables in (s + id)-wave BCS superconductivity in the presence of a weak s wave. We find also a second second-order phase transition. As temperature is lowered past the usual critical temperature T_c, a less ordered superconducting phase is created in the d wave, which changes to a more ordered phase in a (s + id) wave at T_{c1} ($<T_c$). The presence of two phase transitions is manifested by the two jumps in the specific heat at T_c and T_{c1}. The temperature dependencies of the susceptibility, penetration depth, and thermal conductivity also confirm the existence of the new phase transition.

The Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity [1, 2] has been successfully applied to different systems in pure angular momentum states such as s, p, and d waves. However, the unconventional high-T_c superconductors [3] with high critical temperature T_c have a complicated lattice structure with extended and/or mixed symmetry for the order parameter [4]. Some of the high-T_c materials have singlet d-wave Cooper pairs and the order parameter has $d_{x^2-y^2}$ symmetry in two dimensions [4]. Recent measurements [5] of the penetration depth $\lambda(T)$ and superconducting specific heat at different temperatures T and related theoretical analysis [6, 7] also support this point of view. In some cases there is the signature of an extended s- or d-wave symmetry. The possibility of a mixed (s–d)-wave symmetry was suggested some time ago by Ruckenstein *et al* and Kotliar [10]. There is experimental evidence of mixed s- and d-wave symmetry in compounds such as $YBa_2Cu_3O_7$ (YBCO) [8] and $Bi_2Sr_2CaCu_2O_{8+x}$ [9], where an s + exp(iθ)d symmetry is applicable. Recently, this idea has been explored to explain the NMR data for the superconductor YBCO and the Josephson critical current observed in YBCO–SNS and YBCO–Pb junctions [11]. There have also been certain recent theoretical studies using mixed s- and d-wave symmetries [12], and it was noted that a stable mixed s + id state is more likely to be realized than an s + d state, in view of the different couplings and lattice symmetries.

It is quite natural that the Cooper electrons might interact in both s and d waves with different couplings. In the presence of simple central potentials the Cooper problem separates into its decoupled s- and d-wave components. The same decoupling occurs in a linear Schrödinger equation. However, in the non-linear BCS theory, the presence of both s- and d-wave components in the interaction would lead to an order parameter of mixed symmetry and consequently a coupled set of BCS equations. The symmetry of the order parameter is to be specified in order to solve this coupled set of equations.

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The normal state of most high-T_c materials has not been satisfactorily understood, and there are controversies about the appropriate microscopic Hamiltonian and pairing mechanism [4, 7]. Despite this, we study the order parameter in the (s + id)-symmetry case using the weak-coupling microscopic BCS theory based on the Fermi liquid model to extract some model-independent properties of such a description. For a weaker s-wave admixture, quite unexpectedly, we find another second-order phase transition at $T = T_{c1} < T_c$, where the superconducting phase changes from a pure d-wave state for $T > T_{c1}$ to a mixed (s + id)-wave state for $T < T_{c1}$. The specific heat exhibits two jumps at the transition points $T = T_{c1}$ and $T = T_c$. The temperature dependencies of the superconducting specific heat, susceptibility, penetration depth, and thermal conductivity change drastically at $T = T_{c1}$ from power-law behaviour (typical for a d state with node(s) in the order parameter on the Fermi surface) for $T > T_{c1}$ to exponential behaviour (typical for an s state with no nodes) for $T < T_{c1}$. The order parameter for the present s + id wave does not have a node on the Fermi surface for $T < T_{c1}$, and it behaves like a modified/extended s-wave one. The observables for the normal state are closer to those for the superconducting $l = 2$ state than to those for the superconducting $l = 0$ state [7]. Consequently, superconductivity is more pronounced in the s wave than in the d wave. Hence, as the temperature decreases the system passes from the normal state to a 'less' superconducting d-wave state at $T = T_c$ and then to a 'more' superconducting extended s-wave state at $T = T_{c1}$, signalling a second phase transition.

We consider a system of N superconducting electrons under the action of a purely attractive two-electron potential in the partial wave l (=0, 2):

$$V_{\boldsymbol{pq}} = -\sum_{l=0,2} V_l \cos(l\theta_p)\cos(l\theta_q) \tag{1}$$

where θ_p is the angle of the momentum vector $\boldsymbol{p}$.

The potential (1) for an arbitrary, small V_l leads to Cooper pairing instability at zero temperature in even (odd) angular momentum states for the spin-singlet (spin-triplet) state. The Cooper-pair problem for two electrons above the filled Fermi sea is given by [7]

$$V_l^{-1} = \sum_{\boldsymbol{q}(q>1)} \cos^2(l\theta)(2\epsilon_q - \hat{E}_l)^{-1} \tag{2}$$

with the Cooper binding $C_l = 2 - \hat{E}_l$. Here $\epsilon_q = \hbar^2 q^2/2m$ with m the mass of an electron, and the $\boldsymbol{q}$-summation is evaluated according to

$$\sum_{\boldsymbol{q}} \to \frac{N}{4\pi}\int \mathrm{d}\epsilon_q\, \mathrm{d}\theta \equiv \frac{N}{4\pi}\int_0^\infty \mathrm{d}\epsilon_q \int_0^{2\pi} \mathrm{d}\theta. \tag{3}$$

Unless the units of the variables are explicitly mentioned, in this work all energy variables are expressed in units of E_F, such that $T \equiv T/T_F$, $E_{\boldsymbol{q}} \equiv E_{\boldsymbol{q}}/E_F$, $E_F = k_B = 1$ etc, where T_F (E_F) is the Fermi temperature (energy) and k_B is the Boltzmann constant.

We consider a weak-coupling renormalized BCS model in two dimensions with s + id symmetry. At finite T, one has the following BCS equation:

$$\Delta_{\boldsymbol{p}} = -\sum_{\boldsymbol{q}} V_{\boldsymbol{pq}} \frac{\Delta_{\boldsymbol{q}}}{2E_{\boldsymbol{q}}} \tanh\frac{E_{\boldsymbol{q}}}{2T} \tag{4}$$

with $E_{\boldsymbol{q}} = [(\epsilon_q - \mu)^2 + |\Delta_{\boldsymbol{q}}|^2]^{1/2}$. The order parameter $\Delta_{\boldsymbol{q}}$ has the following anisotropic form: $\Delta_{\boldsymbol{q}} \equiv \Delta_0 + \mathrm{i}\Delta_2\cos(2\theta)$ where the Δ_l are dimensionless. The BCS gap is defined by $\Delta(T) = (\Delta_0^2 + \Delta_2^2/2)^{1/2}$, which is the root mean square average of $\Delta_{\boldsymbol{q}}$ on the Fermi surface. Using the above form of Δ_q and potential (1), equation (4) becomes the following coupled set of BCS equations for $l = 0$ and 2:

$$\frac{1}{V_l} = \sum_q \cos^2(l\theta)\frac{1}{2E_q}\tanh\frac{E_q}{2T} \tag{5}$$

where the coupling is introduced through E_q.

Using (2), the set (5) of BCS equations can be explicitly written in terms of Cooper bindings as follows:

$$\int \mathrm{d}\theta\ \cos^2(l\theta)\left[\int_1^\infty \frac{2\ \mathrm{d}\epsilon_q}{2\epsilon_q - \hat{E}_l} - \int_0^\infty \frac{\mathrm{d}\epsilon_q}{E_q}\ \tanh\frac{E_q}{2T}\right] = 0. \tag{6}$$

The two terms in the BCS equation (6) have ultraviolet divergence. However, the difference between these two terms is finite. The BCS model (6) is independent of the coupling V_l, is governed by Cooper binding C_l, and has some advantages [7]. Firstly, no energy cut-off is needed in this equation. This is why model (6) is called renormalized [7, 14]. Secondly, this model leads to an increased T_c in the weak-coupling limit, appropriate for some high-T_c materials [7]. Here, we use the renormalized model for convenience. Otherwise, it has no effect on our conclusions and the same analysis can be performed in the standard BCS model with a cut-off.

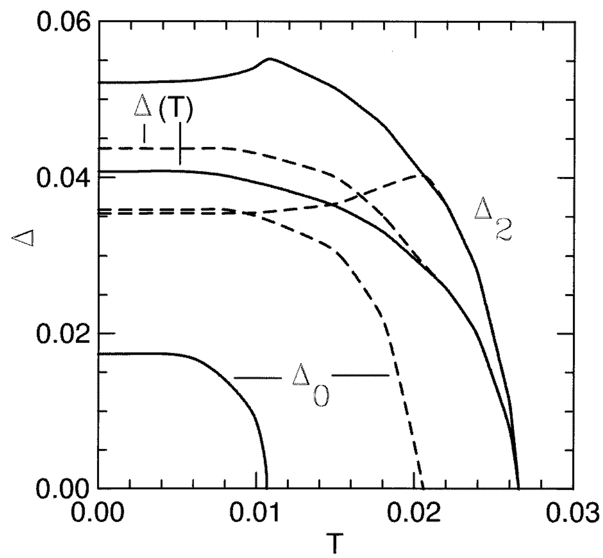

Figure 1. The s- and d-wave parameters Δ_0 and Δ_2, and the BCS gap $\Delta(T)$ at different temperatures for the (s + id)-wave models sd1 (full line) and sd2 (dashed line) described in the text with different mixtures of s and d waves.

The specific heat per particle is given by [2]

$$C(T) = \frac{2}{NT^2}\sum_q f_q(1-f_q)\left(E_q^2 - \frac{1}{2}T\frac{\mathrm{d}|\Delta_q|^2}{\mathrm{d}T}\right) \tag{7}$$

where $f_q = 1/(1+\exp(E_q/T))$. The spin susceptibility χ is defined by [7]

$$\chi(T) = \frac{2\mu_N^2}{T}\sum_q f_q(1-f_q) \tag{8}$$

where μ_N is the nuclear magneton. The penetration depth λ is defined by [2]

$$\lambda^{-2}(T) = \lambda^{-2}(0)\left[1 - \frac{2}{NT}\sum_q f_q(1-f_q)\right]. \tag{9}$$

The superconducting-to-normal thermal conductivity ratio $K_s(T)/K_n(T)$ is defined by [7]

$$\frac{K_s(T)}{K_n(T)} = \left(\sum_q(\epsilon_q - 1)f_q(1-f_q)E_q\right)\Bigg/\left(\sum_q(\epsilon_q-1)^2 f_q(1-f_q)\right). \tag{10}$$

We solved the coupled set of equations (6) numerically and calculated the gaps Δ_0 and Δ_2 at various temperatures for $T < T_c$. The corresponding BCS gap $\Delta(T)$ was also calculated. For a very weak s-wave (d-wave) interaction the only possible solution corresponds to $\Delta_0 = 0$ ($\Delta_2 = 0$). In order to have a coupling between s and d waves, both the interaction potentials have to be reasonable. We have studied the solution only for cases in which a coupling between the two equations is allowed. In this domain we have kept the d-wave coupling stronger than the s-wave coupling, so that as the temperature is lowered past T_c a superconducting phase in the d wave appears. In figure 1 we plot the temperature dependencies of different Δs for two types of s–d mixing corresponding to (1) $C_0 = 0.0006,\ C_2 = 0.001$ (full line) and (2) $C_0 = 0.000\,85,\ C_2 = 0.001$ (dashed line), referred to as models sd1 and sd2, respectively. For a superconductor with $T_F = 5000$ K, the largest of these Cooper bindings C_2 is 5 K. The smallness of this binding guarantees the weak-coupling limit, where the BCS model should provide a good description. In both cases the parameter Δ_2 is suppressed in the presence of a non-zero Δ_0. However, the BCS gap $\Delta(T)$ has the same form as in the case of pure s and d waves. In model sd1 (sd2) $\Delta(0)/T_c = 1.535$ (1.644), $T_c = 0.0266$ (0.0266), $T_{c1} = 0.010\,65$ (0.0206). For a pure s (d) wave, $\Delta(0)/T_c = 1.764$ (1.513) [7]. At $T = 0$ the order parameter has s- and d-wave

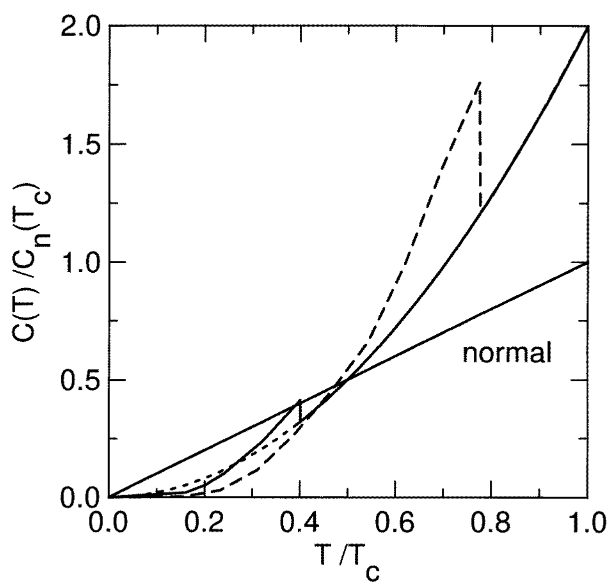

Figure 2. The specific heat ratio $C(T)/C_n(T_c)$ versus T/T_c for models sd1 (full line) and sd2 (dashed line). The dotted line represents the pure d-wave result from reference [7] for comparison.

components, and we find that as T increases both components decrease and for $T \geqslant T_{c1}$ the s-wave component vanishes and one is left with a pure d-wave component, which vanishes at $T = T_c$.

In order to substantiate the claim that there is a second phase transition at $T = T_{c1}$, we study the temperature dependence of the specific heat in some detail. The different specific heats are plotted in figure 2. With this two-step transition, the superconducting specific heat exhibits a very unexpected peculiar behaviour. In both models the specific heat exhibits two jumps—one at T_c and another at T_{c1}. From (7) and figure 1, we see that the temperature derivative of $|\Delta_q|^2$ has discontinuities at T_c and T_{c1} due to the vanishing of Δ_2 and Δ_0, respectively, responsible for the two jumps in the specific heat. For $T_c > T > T_{c1}$, the specific heat exhibits typical d-wave power-law behaviour, $C_s(T)/C_n(T_c) = 2(T/T_c)^2$, as found in recent studies [7]. For $T < T_c$, we find an exponential behaviour. Two jumps in specific heat have been observed recently for certain superconducting compounds, which suggests the existence of a coupled s + id phase [13].

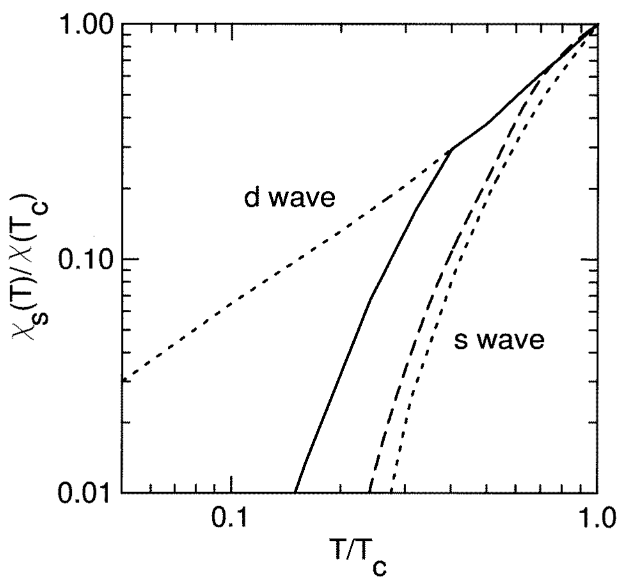

Figure 3. The spin susceptibility ratio $\chi_s(T)/\chi(T_c)$ versus T/T_c for models sd1 (full line) and sd2 (dashed line). The dotted lines represent the pure s- and d-wave results from reference [7], and are given for comparison.

Next we study the temperature dependencies of the spin susceptibility, penetration depth and thermal conductivity, which we exhibit in figures 3–5 where we also plot the results for pure s and d waves from reference [7], for comparison. In all cases, d-wave-type power-law behaviour is obtained for $T_c > T > T_{c1}$. We obtain for the d wave $K_s(T) \approx K_n(T)(T/T_c)^{1.2}$ and $\chi_s(T)/\chi_n(T_c) \approx (T/T_c)^{1.3}$ [7]. For $T < T_{c1}$, there is no node in the present order parameter on the Fermi surface and one has a typical extended s-state behaviour. A passage from a d state to an extended s state at T_{c1} represents an increase in order and hence an increase in superconductivity [7]. As temperature decreases, the system passes from the normal state to a d-wave state at $T = T_c$, and then to an extended s-wave state at $T = T_{c1}$, signalling a second phase transition.

In conclusion, we have studied the (s+id)-wave superconductivity employing a renorm-

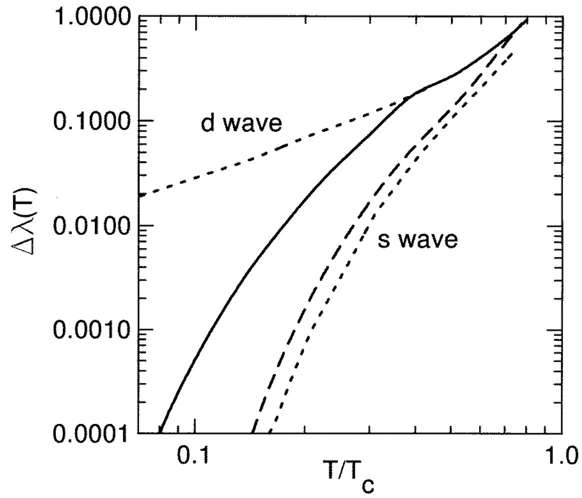

Figure 4. The penetration depth ratio $\Delta\lambda(T) \equiv [\lambda(T) - \lambda(0)]/\lambda(0)$ versus T/T_c for models sd1 (full line) and sd2 (dashed line). The dotted lines represent the pure s- and d-wave results from reference [7], and are given for comparison.

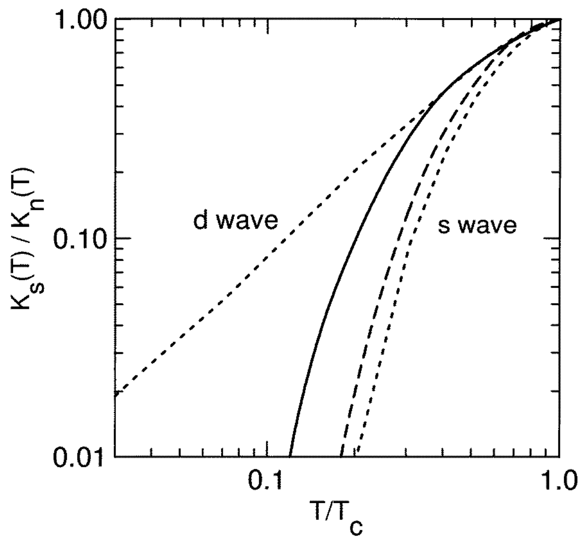

Figure 5. The thermal conductivity ratio $K_s(T)/K_n(T)$ versus T/T_c for models sd1 (full line) and sd2 (dashed line). The dotted lines represent the pure s- and d-wave results from reference [7], and are given for comparison.

alized BCS model in two dimensions, and confirmed the existence of a second-order phase transition at $T = T_{c1}$ in the presence of a weaker s wave. We have kept the s- and d-wave couplings in such a domain that a coupled (s + id)-wave solution is allowed. As temperature is lowered past the first critical temperature T_c, a weaker (less ordered) superconducting phase is created in the d wave, which changes to a stronger (more ordered) superconducting phase in the s + id wave at T_{c1}. The (s + id)-wave state is similar to an extended s-wave state with no node in the order parameter. The phase transition at T_{c1} is also marked by power-law (exponential) temperature dependencies of $C(T)$, $\chi(T)$, $\Delta\lambda(T)$, and $K(T)$ for $T > T_{c1}$ ($<T_{c1}$). A similar second-order phase transition may occur for some other types of mixture of angular momentum states.

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