Comments

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Comment on "Anisotropic superconductors with repulsive average interaction"

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In a recent paper Whitmore and Carbotte concluded that a sufficient condition for the superconducting state to be stable relative to the normal state over a finite temperature range $0 < T < T_c$ is that the attractive part of the effective electron-electron interaction vary over the Fermi surface. We show that this surprising conclusion is not true in general but results from the assumption of a separable attractive interaction.

In the BCS theory[1] of a "weak-coupling" superconductor the linearized gap equation for T infinitesimally below T_c is

$$\Delta(\vec{k}) = \ln\left(\frac{1.13\hbar\overline{\Omega}}{k_B T}\right)\frac{1}{(2\pi)^3} \times \int_{S_F} \frac{dS_{\vec{k}'}}{\hbar|\vec{v}_{\vec{k}'}|} V(\vec{k},\vec{k}')\Delta(\vec{k}') \quad . \tag{1}$$

The effective electron-electron interaction $V(\vec{k},\vec{k}')$ has been cut off at $\pm\hbar\overline{\Omega}$ (a characteristic phonon energy) from the Fermi energy. It has been assumed that the variation of the interaction and the electronic velocity ($\vec{v}$) from one constant energy surface to another is negligible over the energy range of interest so that the wave vectors $\vec{k}$ and $\vec{k}'$ in (1) terminate on the Fermi surface S_F. The superconducting transition temperature T_c is the largest positive T for which a nontrivial solution [i.e., $\Delta(\vec{k}) \not\equiv 0$ of (1) exists].

We convert this homogeneous linear integral equation into a matrix equation by expanding $\Delta(\vec{k}')$ and $V(\vec{k},\vec{k}')$ in terms of the Fermi-surface harmonics introduced by Allen[2]:

$$\Delta(\vec{k}) = \sum_L \Delta_L \Psi_L(\vec{k}) \quad ; \tag{2}$$

$$V(\vec{k},\vec{k}') = \sum_{L,L'} V_{L,L'}\Psi_L(\vec{k})\Psi_{L'}(\vec{k}') \quad . \tag{3}$$

For spin singlet pairing, the only case that we consider, the sum over L in (2) must be restricted so that $\Delta(-\vec{k}) = \Delta(\vec{k})$. We assume that that part of the interaction which determines the gap function can be adequately represented by a finite number of nonzero interaction coefficients $V_{L,L'}$. Substituting (2) and (3) into (1) and making use of the orthonormality condition[2] imposed on the basis functions, we obtain

$$\Delta_L = \ln\left(\frac{1.13\hbar\overline{\Omega}}{k_B T}\right)\sum_{L'} U_{L,L'}\Delta_{L'} \quad , \tag{4}$$

with

$$U_{L,L'} \equiv N(0)V_{L,L'} \quad , \tag{5}$$

where $N(0)$ is the single spin density of states at the Fermi surface. Equation (4) has a solution whenever

$$\det\left|\left[\ln\left(\frac{1.13\hbar\overline{\Omega}}{k_B T}\right)\right]^{-1}\delta_{L,L'} - U_{L,L'}\right| = 0 \quad , \tag{6}$$

i.e., whenever $k_B T = 1.13\hbar\overline{\Omega}\exp(-1/u_i)$ where u_i is the ith positive eigenvalue of the matrix U.

By the expression isotropic (anisotropic) superconductor we shall mean a superconductor in which the gap function $\Delta(\vec{k})$ is (not) constant over the Fermi surface. Usually an interaction $V(\vec{k},\vec{k}')$ is said to be isotropic if it depends on only $|\vec{k}|$, $|\vec{k}'|$, and the angle between $\vec{k}$ and $\vec{k}'$. In this paper we use the term "isotropic" ("anisotropic") interaction to indicate an interaction which is (not) constant as $\vec{k}$ and/or $\vec{k}'$ vary over the Fermi surface. While an isotropic interaction can lead to an anisotropic gap,[3] an "isotropic" or constant interaction cannot. For a separable interaction the terms isotropic and "isotropic" are interchangeable.

As a measure of the "anisotropy" or variation over the Fermi surface of the interaction we use the

quantity

$$A^2 \equiv \frac{\langle\langle V^2(\vec{k},\vec{k}')\rangle_{S_F}\rangle_{S_F'} - \langle\langle V(\vec{k},\vec{k}')\rangle_{S_F}\rangle_{S_F'}^2}{\langle\langle V(\vec{k},\vec{k}')\rangle_{S_F}\rangle_{S_F'}^2} = \frac{\sum_{L,L'} U_{L,L'}^2 - U_{0,0}^2}{U_{0,0}^2} , \quad (7)$$

where the angular brackets with subscript S_F denote a Fermi-surface average.

In the absence of any "anisotropy" in the interaction, $U_{L,L'} = U_{0,0}\delta_{L,0}\delta_{L',0}$ [corresponding to $\psi_0(\vec{k}) \equiv 1$], and we recover the familiar BCS equation

$$k_B T_c = 1.13\hbar\bar{\Omega}\exp(-1/U_{0,0}) ,$$

with $U_{0,0} \equiv N(0)(V_{e\text{-ph}} - V_C)$ for the transition temperature of an isotropic superconductor with attractive phonon-mediated interaction $V_{e\text{-ph}}$ and repulsive Coulomb interaction V_C. For the "isotropic" case $V_{e\text{-ph}}$ must be greater than V_C in order for T_c to be finite.

In the present formalism, the interaction considered by Whitmore and Carbotte[4] is written

$$U_{L,L'} = C_L C_{L'} - N(0) V_c \delta_{L,0}\delta_{L',0} , \quad (8)$$

with $N(0) V_{e\text{-ph}} \equiv C_0^2 > 0$. It is interesting to extend this to include the situation in which the Coulomb interaction is also symmetrically separable:

$$U_{L,L'} = C_L C_{L'} - D_L D_{L'} , \quad (9)$$

with $N(0) V_C \equiv D_0^2 \geq 0$. It is not difficult to show that the largest eigenvalue corresponding to (9) is

$$u_{\max} = \frac{1}{2}\left\{ \sum_L (C_L^2 - D_L^2) + \left[\left(\sum_L (C_L^2 - D_L^2) \right)^2 + 2 \sum_{L,L'} (C_L D_{L'} - C_{L'} D_L)^2 \right]^{1/2} \right\} .$$

Clearly, $u_{\max}$ is nonnegative. A necessary, but not sufficient, condition for it to be zero is that the phonon-mediated and Coulomb interactions have exactly the same "anisotropy" (i.e., $D_L = \gamma C_L$ with γ independent of L so that the second term in the square root vanishes). Barring this exceptional coincidence, the T_c corresponding to an "anisotropic" interaction of the form (9) is finite even if the interaction is repulsive in every (L,L') channel including the (0,0) or "isotropic" channel. This result contains that of Whitmore and Carbotte as a special case ($D_L = 0$ for $L > 0$). They concluded that as long as there is some "anisotropy" or variation over the Fermi surface in the phonon-mediated interaction, no matter how small, then the superconducting state is stable relative to the normal state below some finite transition temperature T_c, even if the average effective electron-electron interaction $V_{e\text{-ph}} - V_C$ is repulsive. This implies that for any crystalline metal the normal ground state is unstable at $T = 0$.

Since it is most unlikely that "anisotropy" in the effective electron-electron interaction in any real material is accurately described by (8) or (9), it is important to see whether or not the above surprising conclusion is true in general. A simple example suffices to show that it is not. Suppose that all the $U_{L,L'}$ are zero except for $U_{0,0}, U_{0,2} = U_{2,0}$ and $U_{2,2}$. In everything that follows the identification of ψ_2 with a particular Fermi-surface harmonic is immaterial provided only that it have the correct symmetry (i.e., even in $\vec{k}$). However, for definiteness, we identify ψ_2 with one of Allen's $N = 2$ harmonics so that we have "s-wave" and "d-wave" channels coupled by an "s-d" interaction. The matrix U now has the nontrivial eigenvalues

$$u_\pm = \frac{1}{2}\{U_{0,0} + U_{2,2} \pm [(U_{0,0} - U_{2,2})^2 + 4U_{0,2}^2]^{1/2}\} .$$

If $U_{0,0} \equiv N(0)(V_{e\text{-ph}} - V_C)$ and $U_{2,2}$ are both negative then $|U_{0,2}|$ must be larger than $\sqrt{U_{0,0}U_{2,2}}$ in order for the maximum eigenvalue u_+ to be positive and hence T_c finite.

In Fig. 1 we illustrate the range of possibilities available for the dependence of T_c on $N(0)V_c$ for $N(0)V_{e\text{-ph}} = 0.28$ and $\hbar\bar{\Omega} = 32$ meV. These parame-

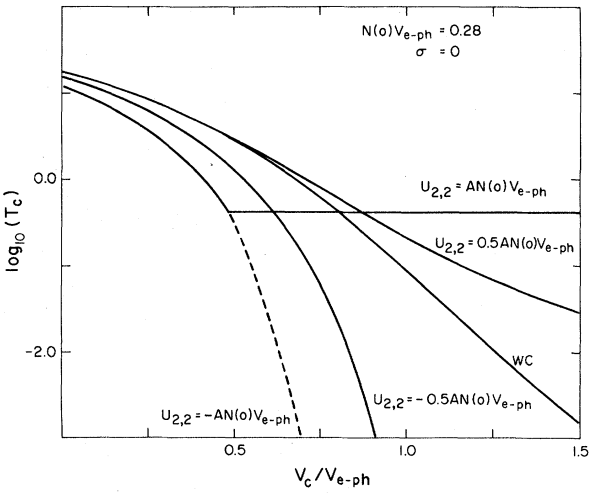

FIG. 1. Variation of the model T_c with $V_C/V_{e\text{-ph}}$ for various choices for the shape of the anisotropy. All curves are for $A^2 = \langle a^2\rangle(2 + \langle a^2\rangle)$ with $\langle a^2\rangle = 0.125$, $N(0)V_{e\text{-ph}} = 0.28$, and $\hbar\bar{\Omega} = 32$ meV.

ters are identical to those used in Fig. 2 of Whitmore and Carbotte.[4] All the curves are for the same value of the anisotropy parameter A^2 and differ only in the relative contributions to A^2 from the "d-wave" channel and "s-d" coupling interactions $U_{2,2}$ and $U_{0,2}$, respectively [see Eq. (7)]. The value used for A^2 corresponds to the largest value of Whitmore and Carbotte's anisotropy parameter $\langle a^2 \rangle$, 0.125, in their Fig. 2. The curve labeled WC is for a separable interaction and is essentially identical to the corresponding curve of Ref. 4. The curves labeled $V_{2,2} = \pm A V_{e\text{-ph}}$ correspond to no "s-d" coupling and hence give T_c curves unaltered from the s wave only solution, except that for $A V_{e\text{-ph}} > V_{e\text{-ph}} - V_C$ the solution corresponds to the d-wave rather than the s-wave state. The other curves show intermediate behavior. For $V_{2,2} = -0.5\, A V_{e\text{-ph}}$ the superconducting solution disappears for V_C only slightly larger than $V_{e\text{-ph}}$ so that the "isotropic" interaction criterion is only slightly altered. On the other hand, for $V_{2,2} = 0.5\, A V_{e\text{-ph}}$ a solution will exist at all values of V_C. For $V_C > V_{e\text{-ph}}$ the solution represents a predominantly d-wave superconducting state which is progressively less strongly coupled with the s-wave state as V_C increases relative to $V_{e\text{-ph}}$. The same observation applies for the separable interaction case.

Markowitz and Kadanoff[5] investigated the effect of nonmagnetic impurities on the transition temperature of a superconductor assuming a separable total effective electron-electron interaction. Whitmore and Carbotte[4] have suggested on the basis of that investigation and their own work that T_c may be extremely sensitive to impurity content for very weak-coupling conductors. We find that their conclusions in this respect are also somewhat distorted by the use of a separable interaction. Extending the analysis of Markowitz and Kadanoff[5] to the general case, represented by Eq. (3), we obtain

$$\Delta_0^{(1)}(\omega) = \Delta_0^{(1)} = \int_0^{\bar{\Omega}} \frac{d\omega'}{\omega'} \tanh\left(\frac{\hbar\omega'}{2k_B T}\right) \sum_{L'} U_{0,L'} \Delta_{L'}^{(1)}(\omega') \,, \tag{10a}$$

$$\Delta_{L\neq 0}^{(1)}(\omega) = \frac{1}{1+(\sigma/\omega)^2} \int_0^{\bar{\Omega}} \frac{d\omega'}{\omega'} \tanh\left(\frac{\hbar\omega'}{2k_B T}\right) \sum_{L'} U_{L,L'} \Delta_{L'}^{(1)}(\omega') \,, \tag{10b}$$

where $\sigma = n_I \langle v_{\vec{k}} \rangle_{S_F} \sigma_s / 2$ with n_I the number of impurities per unit volume and σ_s the impurity cross section assuming pure s-wave scattering. $\Delta_L^{(1)}(\omega)$ is the real part of the complex, frequency-dependent gap coefficient $\Delta_L(\omega)$.

The influence of impurity scattering on T_c implied by these equations is illustrated in Fig. 2 where T_c is plotted versus $V_{2,2}/A V_{e\text{-ph}}$ for various values of σ. The value of A is the same as that used in Fig. 1.

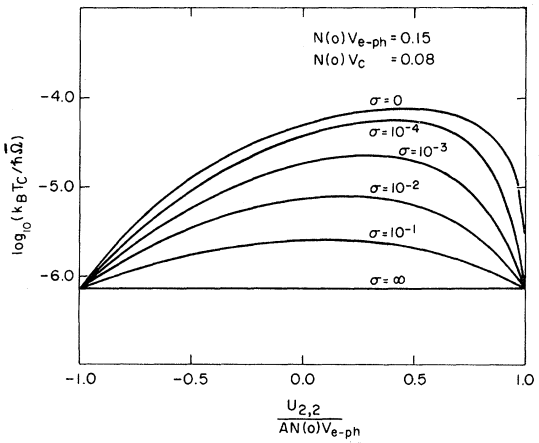

FIG. 2. Dependence of the model T_c on the shape of the "anisotropy" for various values of σ. All curves are for $A^2 = \langle a^2 \rangle (2 + \langle a^2 \rangle)$ with $\langle a^2 \rangle = 0.125$ as in Fig. 1, $N(0) V_{e\text{-ph}} = 0.15$, and $N(0) V_C = 0.08$. The values of σ used to label the various curves are in units of $\hbar\bar{\Omega}$.

The interaction parameters used, $N(0) V_{e\text{-ph}} = 0.15$ and $N(0) V_C = 0.08$, are plausible for the noble metals. Only for materials which have a very low T_c can scattering by nonmagnetic impurities lead to a dramatic change in T_c. The left- and right-hand sides of these curves correspond to placing all of the "anisotropy" in the "d-wave" interaction with no "s-d" coupling while the the separable interaction case places most of the anisotropy in the "s-d" coupling (i.e., $V_{2,2}/A V_{e\text{-ph}}$ is near zero). In the dirty limit $\sigma = \infty$, all anisotropy in the gap is washed out and T_c is determined solely by $V_{0,0}$ so that there is no dependence of T_c on the nature of the "anisotropy" in the interaction. As the impurity scattering is reduced, T_c tends to rise steadily but the rate is strongly dependent on the nature of the "anisotropy." For example, with $V_{2,2} = 0$, T_c increases by about two orders of magnitude in going from the dirty limit to the clean limit, while for $V_{2,2} = \pm A V_{e\text{-ph}}$ there is not "s-d" coupling and T_c is independent of impurity content. (Note, however, that for $V_{2,2} = A V_{e\text{-ph}}$ the "d state" has a higher T_c than the "s state" in the pure limit for the particular choice of parameters considered.) We conclude from this that the separable potential model is likely to overestimate the influence of nonmagnetic impurities on T_c. Nevertheless, it does appear that removal of even nonmagnetic impurities may improve the chances for direct observation of bulk superconductivity in materials with very low superconducting T_c's, as suggested by Whitmore and Carbotte.

In conclusion, we would like to add one further caution against the conclusions drawn in Ref. 4. We believe that the above discussion may be somewhat academic because the starting point, Eq. (1), does not accurately describe real anisotropic superconductors. For the case of weak-coupling superconductors ($|\Delta(\vec{k})|_{T=0}$ is much less than important phonon frequencies) with an "anisotropic" phonon-mediated interaction and an "isotropic" (unrenormalized) Coulomb interaction, the accurate Eliashberg gap equations[6] have been approximated by a much simpler gap equation[7] that gives a reliable description of the anisotropic energy gap at $T=0$. The corresponding equation[7] for T_c can be forced into the form (1) only at the expense of introducing a temperature-dependent interaction that is not symmetric and in $\vec{k}$ and $\vec{k}'$:

$$N(0)V(\vec{k},\vec{k}',T)=\frac{\lambda(\vec{k},\vec{k}')-\mu^*(\Omega_0)-\bar{\lambda}(\vec{k},\vec{k}')/\ln(1.13\hbar\Omega_0/k_BT)}{1+\lambda(\vec{k})}\ , \tag{11}$$

with

$$\lambda(\vec{k},\vec{k}')\equiv 2N(0)\sum_j \frac{|g_{\vec{k},\vec{k}',j}|^2}{\omega_{\vec{k}',\vec{k},j}}\ ,$$

$$\bar{\lambda}(\vec{k},\vec{k}')\equiv 2N(0)\sum_j \frac{|g_{\vec{k},\vec{k}',j}|^2}{\omega_{\vec{k}',\vec{k},j}}\ln\left(1+\frac{\Omega_0}{\omega_{\vec{k}',\vec{k},j}}\right)\ .$$

$\lambda(\vec{k})\equiv\langle\lambda(\vec{k},\vec{k}')\rangle_{S_F}$, $g_{\vec{k},\vec{k}',j}$ is the electron-phonon coupling for the phonon frequence $\omega_{\vec{k}',\vec{k},j}$, and $\mu^*(\Omega_0)$ is the Coulomb pseudopotential. The cutoff for the interaction is Ω_0, the maximum phonon frequency. It has been assumed here, as in Eq. (1), that the cutoff frequency is isotropic. This may not always be a good approximation.

One could obtain a more accurate expression for $V(\vec{k},\vec{k}',T)$ that would be reliable for strong-coupling superconductors as well, by extending the analysis of Dayan and Bar Sagi[8] to the "anisotropic" case. The improved expression would still contain the temperature-dependent $\bar{\lambda}$ term and the unsymmetric factor $[1+\lambda(\vec{k})]^{-1}$. Although these emerge from a careful treatment of the Eliashberg theory they should not, as is sometimes done, be called strong-coupling corrections because this implies that they are important only for strong-coupling superconductors. They are, in fact, more important for weak-coupling materials. To see this, consider an expression[7] for T_c that follows from (1) and (11) provided that $[\Delta(\vec{k})]_{T=T_{c-0^+}}$ contains a nonzero isotropic component $\Delta_{L=0}$:

$$k_BT_c=1.13\hbar\Omega_0\exp\left[-\frac{1+(1+\langle\delta\gamma\rangle)\lambda+(1+\langle\delta\bar{\gamma}\rangle)\bar{\lambda}}{(1+\langle\delta\gamma\rangle)\lambda-\mu^*}\right]\ , \tag{12}$$

with

$$\Delta(\vec{k})\equiv\langle\Delta(\vec{k})\rangle_{S_F}(1+\delta_{\vec{k}})=\Delta_{L=0}(1+\delta_{\vec{k}})\ ,$$

$$\lambda(\vec{k})\equiv\langle\lambda(\vec{k})\rangle_{S_F}(1+\gamma_{\vec{k}})\equiv\lambda(1+\gamma_{\vec{k}})\ ,$$

$$\bar{\lambda}(\vec{k})\equiv\langle\bar{\lambda}(\vec{k})\rangle_{S_F}(1+\bar{\gamma}_{\vec{k}})\equiv\bar{\lambda}(1+\bar{\gamma}_{\vec{k}})\ .$$

$\bar{\lambda}$ cannot be smaller than $(\ln 2)\lambda\approx 0.7\lambda$ and is usually considerably larger than this. To simplify the argument let us assume that $\bar{\lambda}=\lambda$ and that $\langle\delta_{\vec{k}}\bar{\gamma}_{\vec{k}}\rangle_{S_F}=\langle\delta_{\vec{k}}\gamma_{\vec{k}}\rangle_{S_F}$. Then (12) becomes

$$k_BT_c=1.13\hbar\Omega_0\exp\left[-\frac{1}{(1+\langle\delta\gamma\rangle)\lambda-\mu^*}\right]\exp\left[-\frac{2}{1-\mu^*/[(1+\langle\delta\gamma\rangle)\lambda]}\right],$$

where we have split off (to the right) the so-called "strong-coupling" correction factor. For a strong-coupling superconductor, $\lambda>1$, the correction factor is $\sim\exp(-2)$, keeping in mind that $\mu^*\approx 0.1$. For a very weak phonon-mediated interaction, $\lambda(\vec{k},\vec{k}')<\mu^*$, such that T_c is extremely small but finite, we expect $(1+\langle\delta\gamma\rangle)\lambda=(1+x)\mu^*$ with $0<x<<1$. In this case the correction factor is $\sim\exp(-2/x)$. Although Eq. (11) is far from perfect it clearly reveals the futility of using Eq. (1) with a temperature-independent, symmetric interaction to say anything *quantitative* about anisotropic superconductors with ultralow transition temperatures.

In summary, we find that: (i) the BCS gap Eq. (1), with a symmetric temperature-independent interaction, should not be used for quantitative investigations of ansiotropic superconductors, especially if the coupling is very weak; (ii) even assuming this equation, the normal state need not be unstable at $T=0$ for "anisotropic" interactions; and (iii) the dependence of T_c on nonmagnetic impurities can be overestimated by the use of a separable model phonon-mediated interaction in Eq. (1).

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