Effect of interaction anisotropy on the superconducting transition temperature

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(Received 5 October 1994)

We study the influence of pairing interaction anisotropy on the superconducting transition temperature T_c. Our approach involves examining the normal-state instability to Cooper-pair formation using the Bethe-Salpeter equation within a number of simplifying approximations. We make a detailed study of some simple models and find that anisotropy (regardless of its relative strength) has always the effect of increasing T_c. We then consider the generality of this result and find that a general theorem ensures that it holds under rather nonrestrictive assumptions. We discuss the possible implications of our results for superconductivity in real anisotropic materials such as high-temperature superconductors.

I. INTRODUCTION

The calculation from first principles of the superconducting transition temperature T_c is in practice a very difficult problem even in the cases where the pairing mechanism underlying the superconducting state is well understood. It is well known[1] that in elementary versions of the Bardeen-Cooper-Schrieffer (BCS) theory T_c is treated in effect as a free parameter that determines the strength of the modeled superconducting interaction and attention is then focused on dimensionless quantities such as the ratio Δ/T_c (where Δ is the order parameter) which are predicted by the theory. Even in some more sophisticated treatments[2] of standard superconductors, it is apparent that some information about the strength of the electron-phonon coupling is derived from *a priori* knowledge of the transition temperature and that the calculation of T_c has often in it at least a modicum of *a posteriori* element. To put it in a different way, transition temperatures have been often calculated, but seldom predicted.

The extension of the transition temperature range in the past decade has brought a fresh surge of interest in this problem. The obvious question as to why the transition temperatures in the so-called high-temperature superconductors (HTSC's) are so much higher than previously thought possible is rather hard to answer when the calculation of T_c itself is in any case a rather dubious undertaking.

As we shall briefly review below, the difficulties in calculating T_c arise from the exponential sensitivity of the result to the input parameters needed to solve an integral equation. However, these difficulties do not preclude progress if one emphasizes, rather than the value of T_c itself, the identification of factors that cause substantial increases or decreases of T_c in some materials as compared to others. In this way, at least some of the unknown factors can be canceled away in the computation of some appropriate ratio. The *relative* qualitative or semiquantitative trends in the transition temperature as some of the relevant parameters are varied are comparatively much easier to infer, as they can be derived from corresponding variations in the solutions of the appropriate equation. It is then possible to investigate which factors lead, other things being equal, to a higher T_c. This will be our emphasis here.

In this paper we present the results of a study which sheds light on some of the questions introduced in the above paragraphs. A brief account of some of our main results has been previously given.[3] We consider the "Cooper" instability of the Bethe-Salpeter equation and focus our attention specifically on the influence of the pairing interaction anisotropy on the resulting transition temperature. We begin by considering some very simple models within the weak-coupling formalism. We solve these models for the temperature T_c at which the instability occurs and find that, for these examples, the transition temperature obtained for an anisotropic interaction is invariably larger than that obtained for a corresponding isotropic system having the same value of the BCS coupling constant (defined in the usual way as an average over the Fermi surface). We then consider a more general case and formally show that, within some rather nonrestrictive assumptions, it is generally true that anisotropy leads to larger transition temperatures. Furthermore, the numerical results from our models indicate that the increase in T_c arising from anisotropy effects can be quite substantial.

That anisotropy may lead to an increase in T_c has long been part of the lore of superconductivity theory. To our knowledge, the first statement to this effect appears as a nearly incidental remark in a paper[4] dealing with weak anisotropy in the context of studying the effect of impurities in possibly *decreasing* T_c. The effect of weak anisotropy on a variety of properties was subsequently studied mostly in terms of the same separable model po-

0163-1829/95/51(13)/8438(8)/$06.00

tential by other authors.[5,6] While our results agree with these references (and with other previous work as detailed later in the paper) in the appropriate limit, we take here a much more general point of view. Thus, our results are not limited to weak anisotropy, to any particular interaction model, or to a specific partial wave or gap symmetry. We discuss also a new interpretation of gap anisotropy as being possibly connected to a broken symmetry in the system.

Anisotropy is, of course, a salient characteristic of most HSTC's and it is well known that there is often a correlation among HTSC's within the same "family,"[7] between T_c and the degree of anisotropy. This has been an important part of the motivation for this work. However, we caution the reader that, while our conclusions are in our opinion highly suggestive as to some possibilities for high-temperature superconductivity, one should nevertheless keep in mind that the models and formalism discussed here are clearly too oversimplified to be an accurate description of these materials. In addition, there are additional factors not studied here, such as the effect of momenta[8] and frequency dependence[9] of the interaction away from the Fermi surface, which are known to have a strong influence on T_c. These and other considerations must be kept in mind. Nevertheless, there is a considerable degree of generality in our argument that makes it more likely that our results have relevant implications for these and possibly other physical systems.

After this Introduction, we discuss in the next section our formalism and some model examples. In Sec. III, we turn to more general results and discuss our conclusions. We show that the results obtained from the models studied in Sec. II have a wide range of validity, and suggest an additional interpretation of the extended results as representing a possible broken symmetry effect in the interaction mechanism.

II. FORMALISM AND EXAMPLES

A. General considerations

Although the transition temperature can be calculated in elementary cases from the gap equation (by finding the temperature at which the gap vanishes) it is far more convenient in general[10] to calculate T_c from the properties of the normal phase by finding the temperature at which a pairing instability in the Bethe-Salpeter[11] equation for fermion-fermion scattering occurs in the appropriate channel. This instability in the ground state of the Fermi liquid leads to the formation of Cooper pairs. For many simple cases, study of this instability leads to an expression for T_c of the McMillan[12] form

$$T_c = 1.134\alpha\omega_0 \exp(-1/\lambda_{\text{eff}}), \tag{2.1}$$

where ω_0 is a cutoff frequency and α a number of order unity.[13] In the BCS model one has $\alpha = 1$, ω_0 is identified with the Debye frequency, and λ_{eff} is simply λ, the dimensionless electron-phonon coupling constant of the model. For many ordinary superconductors one has[12] the generalization $\lambda_{\text{eff}} = [\lambda - \mu(1 + 0.62\lambda)]/[1.04(1 + \lambda)]$, where μ is a dimensionless measure of the Coulomb repulsion. It is also worth noting[14] that the numerical solution of the Bethe-Salpeter equation for liquid ^{3}He within the spin fluctuation model can be fitted to the form (2.1). The pervasive form of the above eqation is a good illustration of the difficulties that arise in the calculation of T_c: The result depends exponentially on the input parameters needed to solve an integral equation.

In Fig. 1 we show schematically the Bethe-Salpeter (BS) equation, which for our purposes can be conveniently written as

$$\Gamma(\mathbf{k},\mathbf{k}') = V(\mathbf{k},\mathbf{k}') + \sum_{\mathbf{k_1}}\sum_{\omega} V(\mathbf{k},\mathbf{k_1})G(\mathbf{k_1},\omega) \times G(-\mathbf{k_1},-\omega)\Gamma(\mathbf{k_1},\mathbf{k}'), \tag{2.2}$$

where, within weak coupling, $G(\mathbf{k},\omega)$ is a free fermion Green's function and the ω are Matsubara frequencies. In (2.2), $V(\mathbf{k},\mathbf{k}')$ is the effective pairing interaction (which we assume throughout this paper to be frequency independent) and Γ the vertex function. T_c is the highest temperature at which Γ as depicted in Fig. 1 diverges.

We now make the following additional assumptions, which permit us to drastically simplify Eq. (2.2). We will relax some of these assumptions in the next section. First, we assume that V vanishes unless the energies corresponding to the fermions with wave vectors $\mathbf{k}$ and $\mathbf{k}'$ are within an energy range ω_0 about the Fermi surface, with $\omega_0 \ll \epsilon_F$, where ϵ_F is the Fermi energy. Next, we take the Fermi surface to be spherical (or circular if the system is two dimensional). Finally, we consider a simple parabolic band characterized by a single effective mass. With these rather drastic assumptions, it is easy to find the instabilities of Γ as given by Eq. (2.2). Consider first the case where the pairing interaction is isotropic. Then, one can expand[15] in terms of Legendre polynomials:

$$V(\mathbf{k},\mathbf{k}') = \frac{1}{N(0)}\sum_{\ell} U_\ell(2\ell+1)P_\ell(\cos\gamma), \tag{2.3}$$

where γ is the angle between $\mathbf{k}$ and $\mathbf{k}'$, $N(0)$ is the density of states at the Fermi surface, and the P_ℓ are Legendre polynomials. Similarly,

$$\Gamma(\mathbf{k},\mathbf{k}') = \frac{1}{N(0)}\sum_{\ell} \Gamma_\ell(2\ell+1)P_\ell(\cos\gamma). \tag{2.4}$$

Then, the radial integrals in (2.2) are elementary[1] and one has the solution

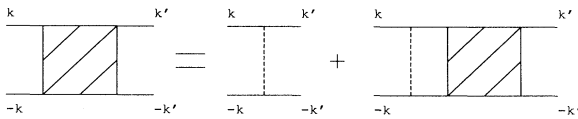

FIG. 1. Schematics of the Bethe-Salpeter equation. Dashed lines represent interactions, and solid lines fermion propagation. Shaded squares represent the vertex function Γ.

$$\Gamma_\ell = \frac{U_\ell}{1 + X(0)U_\ell}, \tag{2.5}$$

where $X(0) = -N(0)\ln(1.134\omega_0/T)$. One obtains then the well-known result that T_c is determined by the most attractive of the U_ℓ. (We employ here the common convention in superconductivity of taking the attractive coupling constants as being positive.) In the ordinary BCS case this is U_0, which equals the averaged interaction over the Fermi surface, and one recovers from (2.5) the usual BCS formula for T_c, of the form in Eq. (2.1) with a bare $\lambda = U_0$. In ^{3}He it is the $\ell = 1$ coupling constant which turns out to be most dominant.

Consider now the case where the interaction is anisotropic. Then, one cannot expand in Legendre polynomials but there are still several methods one can use to solve the BS equation. One can, in many cases, solve (2.2) by iteration, or by performing a double expansion. Here we use the second procedure, although we have double checked the results with the iteration method. For an anisotropic interaction a double expansion in terms of spherical harmonics is still valid:

$$V(\mathbf{k},\mathbf{k}') = \frac{4\pi}{N(0)} \sum_{\ell,m,\ell',m'} U_{\ell m}^{\ell' m'} Y_\ell^m(\hat{\mathbf{k}}) Y_{\ell'}^{m'*}(\hat{\mathbf{k}}') \tag{2.6}$$

and, similarly, for the vertex function,

$$\Gamma(\mathbf{k},\mathbf{k}') = \frac{4\pi}{N(0)} \sum_{\ell,m,\ell',m'} \Gamma_{\ell m}^{\ell' m'} Y_\ell^m(\hat{\mathbf{k}}) Y_{\ell'}^{m'*}(\hat{\mathbf{k}}'). \tag{2.7}$$

These expansions are not immediately useful because the BS equation is no longer, in general, diagonal in terms of spherical harmonics. However, in all physical cases the matrix $\hat{U}$ whose matrix elements are the expansion coefficients in Eq. (2.6) (with each pair ℓ, m labeling the rows and ℓ', m' the columns) will be diagonalizable. Then it follows from the linear structure of (2.2) that the corresponding matrix $\hat{\Gamma}$ is diagonal in the same representation as $\hat{U}$. If we denote by U_α the eigenvalues of $\hat{U}$, with the functions $\langle\hat{\mathbf{k}}|\alpha\rangle$ being the corresponding normalized eigenfunctions, then the solution to (2.2) is given by

$$\Gamma(\mathbf{k},\mathbf{k}') = \frac{4\pi}{N(0)} \sum_\alpha \Gamma_\alpha \langle\hat{\mathbf{k}}|\alpha\rangle \langle\hat{\mathbf{k}}'|\alpha\rangle^*, \tag{2.8}$$

where the eigenvalues of $\hat{\Gamma}$ are given by

$$\Gamma_\alpha = \frac{U_\alpha}{1 + X(0)U_\alpha}, \tag{2.9}$$

where $X(0)$ is as defined below (2.5). The transition temperature is determined simply by the largest positive eigenvalue of $\hat{U}$. We will denote this largest eigenvalue by λ_0 in this work. Thus we have

$$T_c = 1.134\omega_0 e^{-1/\lambda_0}. \tag{2.10}$$

If this eigenvalue is nondegenerate, then the symmetry of the order parameter immediately below T_c is determined by the corresponding eigenfunction. If it is degenerate, the symmetry of the order parameter cannot be determined from the above considerations, although it might be determined[16,17] from a study of the Ginzburg-Landau region. In two dimensions, a similar result is obtained by expanding in terms of planar harmonics.

It is of course relevant to compare these results with the corresponding ones in the isotropic case. Consider first the s-wave state which is obtained in the usual version of the BCS theory after first averaging the interaction over the Fermi surface so as to deal with a single coupling constant. By performing this average in the interaction (2.6) one immediately obtains

$$T_c^{\mathrm{BCS}} = 1.134\omega_0 e^{-1/\lambda^{\mathrm{BCS}}}, \tag{2.11}$$

with

$$\lambda^{\mathrm{BCS}} = U_{0,0}^{0,0}. \tag{2.12}$$

For higher partial waves the definition of a "BCS" coupling constant is less unambiguous. A consistent definition is obtained by multiplying (2.6) by $P_\ell(\cos\gamma) = [4\pi/(2\ell+1)]\sum_m Y_\ell^m(\hat{\mathbf{k}}) Y_\ell^{m*}(\hat{\mathbf{k}}')$ and then averaging over angles. In this way one obtains a "BCS" isotropized transition temperature for the ℓ partial wave given by the form (2.11) with λ^{BCS} replaced by $\lambda_\ell^{\mathrm{BCS}}$:

$$\lambda_\ell^{\mathrm{BCS}} = \frac{1}{2\ell+1} \sum_m U_{\ell,m}^{\ell,m}. \tag{2.13}$$

For an isotropic interaction, one recovers from (2.13) the standard result[17,18] for the BCS coupling constant in each partial wave. In that case, one will always have that the largest $\lambda_\ell^{\mathrm{BCS}}$ equals λ^0, since the interaction matrix is then diagonal in ℓ and independent of m.

B. Simple example: Perturbation theory

To explore the implications of these results, let us consider first a very simple example. Let us study, in two dimensions, the interaction

$$V(\mathbf{k},\mathbf{k}') = \frac{V_0}{1 + a(k_x - k_x')^2 + b(k_y - k_y')^2}, \tag{2.14}$$

where V_0 is a positive (attractive) dimensionless constant, the interaction strength in units of $N(0)$ for this example, and a and b are constants (which we take to be positive). The wave vectors are assumed to be given in units of k_F, the Fermi wave vector, so that a and b are dimensionless. The interaction (2.14) can be given a physical interpretation as some screened boson-mediated interaction. In the limit $a = b$ it is isotropic.

As discussed in the previous subsection, we assume that the wave vectors in (2.14) are on the Fermi circle. Then, we consider the expansion of V in planar harmonics:

$$V(\mathbf{k},\mathbf{k}') = \frac{1}{N(0)} \sum_{m,m'} U_{m,m'} e^{im\phi} e^{-im'\phi'}, \tag{2.15}$$

where ϕ and ϕ' are the azimuthal angles defining the vectors $\mathbf{k}$ and $\mathbf{k}'$ on the Fermi circle. In the limit $a = b$, this interaction is trivially diagonal and one has (see the Appendix)

$$U^{(0)}_{mm'} = \delta_{m,m'} \frac{V_0}{2b \sinh \psi} e^{-m\psi}, \tag{2.16}$$

where ψ is defined by $\cosh \psi \equiv (1 + 2b)/(2b)$. It follows from (2.16) and the two-dimensional version of (2.5) that pairing will be, in the isotropic case, in the s wave.

In the general case, it is not easy to obtain the elements of the matrix $\hat{U}$, defined by (2.15), in closed form. Therefore we will discuss here the case where the anisotropy is small, $b \approx a$, and expand in the small dimensionless parameter, $\delta \equiv b - a$, to lowest nontrivial (second) order.

In the language of the previous subsection, the largest eigenvalue of the zeroth-order (in δ) approximation to the matrix $\hat{U}$ is that corresponding to $m = 0$. We now want to see how the anisotropy perturbs this eigenvalue. This is straightforward, using standard perturbation theory techniques.[19] All of the necessary integrals can be done using complex variable methods. Some details are given in the Appendix. One obtains the result

$$\lambda_0 = U^{(0)}_{0,0} + U^{(1)}_{0,0} + U^{(2)}_{0,0} + \Delta\lambda_0, \tag{2.17}$$

where the first term on the right side is the zeroth-order part as given in (2.16). The next two terms are the diagonal corrections corresponding, respectively, to the first- and second-order terms in the expansion of V, as discussed in the Appendix:

$$U^{(1)}_{0,0} = -\frac{V_0 \delta}{(2b)^2} \frac{(1 - \cosh \psi)}{\sinh^3 \psi}, \tag{2.18}$$

$$U^{(2)}_{0,0} = V_0 \frac{\delta^2}{(2b)^3} \frac{9}{4} \frac{(\cosh \psi - 1)^2}{\sinh^5 \psi}, \tag{2.19}$$

and, finally, $\Delta\lambda_0$ is the second-order correction due to coupling between off-diagonal first-order matrix elements. It follows from the discussion in the Appendix that this term involves only couplings to the d-wave state, and is given by

$$\Delta\lambda_0 = \frac{\delta^2 V_0}{16 b^3} \frac{e^{-2\psi} \sinh \psi}{1 - e^{-\psi}} \left(\frac{1}{\sinh \psi} - \frac{\cosh \psi (\cosh \psi - 1)}{\sinh^3 \psi} - \frac{1}{1 + \cosh \psi} \right)^2. \tag{2.20}$$

That this correction arises from coupling to the d-wave state, rather than the p-wave state, is related to the fact that the model interaction is spin independent, and therefore will not mix singlet and triplet states. The eigenvector corresponding to the eigenvalue in (2.17) is a linear combination of s and d states, consistent with the fact that m is no longer a good quantum number for the problem. The coefficients of the linear combination can easily be found from textbook formulas.

The transition temperature is now given by combining (2.10) and (2.17). We want to compare this result with the corresponding one in the isotropic case, to the same order. From (2.12) and the above calculations, it follows that

$$\lambda^{\mathrm{BCS}} = U^{(0)}_{0,0} + U^{(1)}_{0,0} + U^{(2)}_{0,0} = \lambda_0 - \Delta\lambda_0. \tag{2.21}$$

Now, it is readily seen from (2.20) that the quantity $\Delta\lambda_0$ is positive definite. Therefore one has $\lambda_0 \geq \lambda^{\mathrm{BCS}}$, and consequently $T_c \geq T_c^{\mathrm{BCS}}$, with the equality applying only in the limit $a = b$. Thus, the anisotropy always leads to an increase in the transition temperature: For this model, an anisotropic system will always have a larger T_c than an isotropic system having the same value of the pairing interaction averaged over the Fermi surface. The fact that the lowest-order correction to λ^{BCS} goes as δ^2 agrees with what was found in Ref. 4 for the separable weakly anisotropic model potential[4–6] $V = V_0[1+a(\hat{\mathbf{k}})][1+a(\hat{\mathbf{k}}')]$ (where a is small).

C. Exactly solvable model

One might suspect that the final result for the model in the previous subsection would be valid only in perturbation theory. Indeed, that the off-diagonal second-order correction to the largest or smallest eigenvalue of a given operator has a definite sign follows from the form of the perturbation theory itself.[19] To check that this is not the case, we consider here a simpler model that can be solved exactly.

We will work now in three dimensions with the interaction given by

$$V(\mathbf{k}, \mathbf{k}') = V_0[1 + a(k_x - k'_x)^2 + b(k_y - k'_y)^2 + c(k_z - k'_z)^2], \tag{2.22}$$

where again V_0 is the strength of the interaction in units of $N(0)$, the momenta are in units of k_F, and a, b, and c are dimensionless constants. We make no assumption as to their signs in this case. Although the physical interpretation of the interaction (2.22) is not as straightforward as that of (2.14), one can see that it is not unphysical in real space. The main advantage of this model is that it can be solved easily and exactly and therefore it will help us understand the significance of the previous results in a nonperturbative setting. We will also be able to investigate triplet pairing states. The interaction (2.22) is isotropic in the limit $a = b = c$. One can consider also the particular case $a = b \neq c$ where the anisotropy is limited to the z direction, as was done in Ref. 3.

Once again, we assume that all relevant wave vectors are on the Fermi surface, so that the interaction (2.22) can be rewritten in terms of the polar and azimuthal angles of $\mathbf{k}$ and $\mathbf{k}'$. It is then straightforward to rewrite (2.22) in terms of spherical harmonics, and thus obtain the matrix elements $U^{\ell' m'}_{\ell m}$ defined in (2.6). Only the range of values $\ell \leq 2$, $\ell' \leq 2$ appears since no powers of the sine or cosine higher than two are present. Therefore the matrix $U^{\ell', m'}_{\ell, m}$ [see (2.6)] is fairly small in size.

Further, since the interaction is spin independent, singlet and triplet states (even and odd values of ℓ and ℓ') again decouple and one obtains separate 4×4 and 3×3 matrices for the two cases. The only nonvanishing matrix elements for the singlet subspace are found to be

$$U_{0,0}^{0,0} = 1 + (2/3)(a+b+c), \quad U_{0,0}^{2,0} = \frac{1}{3\sqrt{5}}(2c-a-b),$$
$$U_{0,0}^{2,2} = U_{0,0}^{2,-2} = \frac{1}{\sqrt{30}}(a-b), \tag{2.23}$$

plus those obtained by interchanging $\ell \leftrightarrow \ell'$ and $m \leftrightarrow m'$. For the triplet subspace one similarly has

$$U_{1,0}^{1,0} = -(2/3)c, \quad U_{1,1}^{1,1} = U_{1,-1}^{1,-1} = -(1/3)(a+b),$$
$$U_{1,1}^{1,-1} = -(1/3)(a-b). \tag{2.24}$$

It is now straightforward to find the eigenvalues and eigenvectors. We tackle first the singlet case. There are four eigenvalues, but two are trivially zero. Introducing the auxiliary quantity β,

$$\beta^2 = (U_{0,0}^{2,0})^2 + 2(U_{0,0}^{2,2})^2, \tag{2.25}$$

we have for the two nontrivial eigenvalues

$$\lambda_\pm = (1/2)[U_{0,0}^{0,0} \pm \sqrt{(U_{0,0}^{0,0})^2 + 4\beta^2}]. \tag{2.26}$$

We see that $\lambda_+ \geq \lambda_-$, and therefore we have, if singlet pairing is favored, that $\lambda_0 = \lambda_+$ as given in (2.26). The corresponding eigenvector, as seen from the form of the submatrix defined by (2.23), is a linear combination of $\ell = 0$ and $\ell = 2$ states, specifically,

$$\langle \hat{\mathbf{k}}|0\rangle = \alpha_+ Y_0^0(\hat{\mathbf{k}}) + \beta_+ Y_2^0(\hat{\mathbf{k}}) + \gamma_+[Y_2^2(\hat{\mathbf{k}}) + Y_2^{-2}(\hat{\mathbf{k}})], \tag{2.27}$$

where

$$\alpha_+ = \frac{1}{D}, \qquad \beta_+ = \frac{U_{0,0}^{2,0}}{D},$$
$$\gamma_+ = \frac{U_{0,0}^{2,2}}{D}, \qquad D \equiv \sqrt{(\lambda_+)^2 + \beta^2}. \tag{2.28}$$

On the other hand, the BCS coupling constant is given by (2.12) and the first of (2.23). It follows then immediately from (2.26) that we have also here

$$\lambda_0 \geq \lambda^{\mathrm{BCS}} \tag{2.29}$$

and this is no longer merely a perturbative result.

A similar situation occurs for triplet pairing ($\ell = 1$). The three eigenvalues of the matrix with nonzero matrix elements as given in (2.24) are

$$\lambda_a = -(2/3)a, \qquad \lambda_b = -(2/3)b, \qquad \lambda_c = -(2/3)c. \tag{2.30}$$

The corresponding eigenvector for λ_c is the Y_1^0 spherical harmonic, while those corresponding to λ_a and λ_b are linear combinations of Y_1^1 and Y_1^{-1}. If one of the constants a, b, c, is large and negative (the "repulsive" sign) we still get a finite T_c, although in the $\ell = 1$ channel. That a strong repulsive anisotropic interaction may lead to pairing was pointed out in Ref. 20.

The corresponding BCS coupling constant as given by (2.13) is

$$\lambda_1^{\mathrm{BCS}} = -(2/9)(a+b+c), \tag{2.31}$$

which can never be larger than the largest of the eigenvalues in (2.30). Hence, we are led again to a result of the form (2.29).

Numerically, the increases in T_c resulting from the anisotropy can easily be very considerable, because of the strong dependence of T_c on the coupling constant. Let us focus on the singlet case for some numerical examples. Assume, for example, $\omega_0 = 300$ K, $a = b = 1$, $c = -1$, and a BCS transition temperature of 3 K. From (2.12) and (2.23), we can obtain the BCS coupling constant, which gives us the value of the strength V_0 in (2.22). On the other hand, using this value of V_0 and the same values of the other parameters we find that the exact transition temperature as given by (2.10) [with λ_0 as in (2.26)] is 4.91 K. If we decrease the value of c, $c = -2$, then we get $T_c = 15.2$ K. With $\omega_0 = 600$ K and the previous values for the potential parameters, we get an increase in T_c from 20 K to 67 K. Examples of much larger increases can easily be found, in both the singlet and triplet cases, although the results must be viewed as only indicative, since they are then beyond the weak-coupling limit.

Finally, the two-dimensional version of the model (2.22) can of course also be solved exactly, with the same conclusions. In that case, and with $a \neq b$, the singlet state is, as in Sec. II B, a linear combination of s and d states.

III. GENERAL RESULTS AND DISCUSSION

The results of the previous section are a strong indication that anisotropy in the pairing interaction has a favorable effect on the transition temperature. To be more precise, we have shown the following, for the models studied there: Consider two systems with the same form for the pairing interaction [e.g., both with pairing interactions of the form (2.14) or the form (2.22)] but with different values of the parameters controlling the degree of anisotropy. Let us, for definiteness, assume that both undergo pairing in the s wave (similar considerations apply to the other partial waves in our last example). Assume then that the two systems are such that they both have the same value for the *average* of the pairing interaction over the Fermi surface, which means that they have the same value for the BCS coupling constant, but that the interaction for the first system is isotropic, while that for the second system is not. In the language of the previous section, both systems have the same value of $U_{0,0}^{0,0}$ (or $U_{0,0}$ in the two-dimensional case) but only the first system is diagonal in the spherical (or planar) harmonic basis. Then, we have shown that the second system will

have a superconductiong transition temperature higher than the first. It is in this sense that our arguments indicate that pairing is favored by anisotropic interactions.

It is natural at this point to approach the question of the generality of our results. At the level of the assumptions we have considered in this work, it is easy to see that our results are very general. In effect, we have that the BCS coupling constant is given [see (2.12)] as a diagonal matrix element[21] of $\hat{U}$, while the exact coupling constant is the largest eigenvalue. But, assuming only that the spectrum of $\hat{U}$ is bounded from above, it follows immediately that its largest eigenvalue, which we have denoted by λ_0, cannot be smaller that the largest of all the diagonal elements. This result, which for finite matrices is one of the basic theorems related to Rayleigh's quotient,[22] can be seen most easily from the variational method: Let $|u\rangle$ be a normalized trial vector in the Hilbert space of fermionic pairing states, and consider its expansion in terms of the eigenstates $|\alpha\rangle$ as defined in the paragraph below (2.7):

$$|u\rangle = \sum_{\alpha} a_{\alpha}|\alpha\rangle. \tag{3.1}$$

One then has

$$\langle u|U|u\rangle = \sum_{\alpha} \lambda_{\alpha}|a_{\alpha}|^2 \leq \lambda_0, \tag{3.2}$$

where the λ_α are the eigenvalues, and we have, in the last step, made use of the state normalization. If one takes for the trial state $|u\rangle$ any state in the original basis (the spherical harmonics in our case), one has the proof of the Rayleigh's quotient statement cited above. Thus, the situation found in the previuos examples is actually a general property.

Having made this point, we can now go on to consider the effect of removing some of the assumptions made in order to derive our previous results. Let us begin with removing the assumption that the Fermi surface is spherical, and that the crystallographic structure of the material is not relevant. In general, we could then still assume that all angular dependences can be expanded in terms of the complete set of spherical harmonics, while the radial dependence of the interaction is through the energy, and can be dropped if all wave vectors are still on the Fermi surface, whatever its shape. This point of view would lead straightforwardly to a formal extension of the validity of the results. However, we will take an alternative point of view, involving more general, although maybe more speculative, considerations, and a somewhat different concept of what anisotropy means.

When considering a nonspherical Fermi surface, it is often convenient to expand in the appropriate complete set of functions related to the crystal symmetry group[23] as the spherical harmonics are related to the rotation group. These functions determine in principle the possible symmetries of the order parameter, which have been sorted out[24] for the symmetry groups corresponding to high-T_c superconductors. Let us denote these functions as $\varphi_i(\hat{\mathbf{k}})$ and the corresponding states simply as $|i\rangle$. Consider now the matrix $\hat{V}$ of the pairing interaction in the basis set of these functions $\varphi_i(\hat{\mathbf{k}})$. Expanding also the vertex function Γ in terms of the states $|i\rangle$, one can formally solve the BS equation in terms of those states and conclude again that the largest attractive eigenvalue of $\hat{V}$ determines the transition temperatures as in (2.10). Then, the same proof leading to Eq. (3.2) shows that an anisotropic system, in the sense of one in which the matrix $\hat{V}$ is not diagonal, leads to a higher T_c than one in which this matrix is diagonal.

We have introduced, in the last paragraph, a subtly different version of the meaning of "anisotropic," which earlier in the paper simply meant "not invariant under rotations." In the last paragraph we are considering it with the meaning of "having a lower-symmetry than the crystal structure." It is only under this second meaning that the full generality of our conclusion as derived from the statement (3.2), which in plain language is that anisotropy favors superconductivity, applies. It is obvious that off-diagonal pairing interactions in the sense just described are quite unusual, if indeed they exist at all. Ordinary phonon interactions have, of course, the symmetry of the lattice. But it is possible for a system to have, for example, a magnetic instability with a symmetry lower than that of the lattice. Thus, one can in principle imagine an exotic, electronic pairing mechanism involving lower-symmetry antiferromagnetic fluctuations that would have this property. It is even possible to imagine a phononic mechanism having this property in a system which is simultaneously near a superconducting and a structural instability.[25] In effect, we are saying that this kind of *broken symmetry* would always lead to an increase in T_c.

We have used a weak-coupling form (bare electron propagators) of the Bethe-Salpeter equation in this work. Strong-coupling effects were considered in a previous separable model[6] in the weak-anisotropy limit. More recently, the interplay of strong-coupling effects and anisotropy was studied by Combescot,[26] who found that, because of mass renormalization effects, strong coupling suppresses anisotropy. It therefore would tend to diminish anisotropy related T_c enhancement. However, HTSC's remain strongly anisotropic even though the coupling is presumably not weak. On the other hand, the interplay of anisotropy with Coulomb repulsion effects may well lead[27] to further increases in T_c. Therefore, although the results would depend on the precise details of the strong-coupling interaction, we believe that even if inclusion of strong-coupling effects may diminish the generality of our results, there would still be a wide range of circumstances where our main qualitative conclusions would apply. It is most unlikely that lifting the restrictions imposed by our assumptions would invariably lead to the general invalidation of our results. One reason for this is the ubiquity of (2.1), that is, of the exponential dependence of T_c on the effective coupling strength. We have found that anisotropy increases the bare coupling strength by bringing in a contribution from a different partial wave (symmetry state). In the strong-coupling case, the net effect will depend also on how this contribution influences the effective mass renormalization or

repulsive effects. In any case it does not seem to us likely that the increase in the bare coupling would be invariably canceled away. Another reason is the physical interpretation of our result: By allowing anisotropy, one in effect introduces additional degrees of freedom in the problem and, because of the variational nature of BCS theory, this increase will lead in general to higher transition temperatures. Our results have been obtained in the clean limit. Impurities might tend to diminish anisotropy effects and consequently partly negate the T_c enhancement, but any such effect should not affect, e.g., HTSC's where the coherence length is smaller than the mean free path.

One can at this point only speculate whether these considerations have any relevance to real materials or, in particular, to HTSC's. The enhancement in T_c found in deformed[28] Ti-Mo structures and in[29] In under uniaxial stress might be related to our ideas although experimental evidence[30] on HTSC crystals under uniaxial pressure is ambiguous. A combination of s and d two-dimensional states not dissimilar to that obtained in the perturbation model of Sec. II B or the two-dimensional version of (2.22) remains a leading candidate to explain the many apparently divergent experimental results (see, e.g., Refs. 31 and 32) on the pairing state of HTSC's. Several of the high-temperature mechanisms for superconductivity that have been proposed (see for example Refs. 8 and 9) do enlarge the configurational space for the order parameter by considering explicitly its dependence on quantities away from the Fermi surface. Variational considerations such as those presented above show that such an expansion of the relevant Hilbert space *cannot* lead to a decrease in T_c, and of course usually will lead to an increase. We therefore consider it likely that, in some sense, an ingredient of this kind will be present in the ultimate explanation of the mechanism of high-temperature superconductivity. It is obvious, nevertheless, that the speculations presented in these last paragraphs are insufficient to determine the precise nature of this ingredient.

ACKNOWLEDGMENTS

This work has been supported in part by NATO Grant No. CRG94005. O.T.V. thanks the members of the Orsay theory group for their hospitality. We thank B.P. Stojković for a careful reading of the manuscript. M.T.B-M. thanks R. Combescot for an interesting discussion on Ref. 3, in which he brought some of the previous work on the subject to her attention, and J.P. Contour and J. Demoment for enjoyable discussions.

APPENDIX A: EXPANSIONS

We briefly discuss here the integrals required in the computations of Sec. II.

In terms of the azimuthal angles ϕ and ϕ' and the dimensionless parameters b and $\delta \equiv b-a$, the interaction (2.14) can be written as

$$V(\phi,\phi') = \frac{V_0}{1+2b[1-\cos(\phi-\phi')]-d(\cos\phi-\cos\phi')^2}, \tag{A1}$$

which can be expanded as indicated in (2.15). Consider first the zeroth-order result of Eq. (2.16). One has

$$U^{(0)}_{m,m'} \propto \int_0^{2\pi} d\phi \frac{e^{im\phi}}{\cosh\psi-\cos\phi} \tag{A2}$$

[recall that ψ is defined below (2.16)], which is trivially done by contour integration after the change $z = \cos\phi$. The evaluation of the second-order terms [Eqs. (2.18), (2.19), and (2.20)] involves evaluation of the integrals

$$I^{p,q}_{m,m'} = \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi' e^{im\phi} e^{-im'\phi'} \frac{(\cos\phi-\cos\phi')^p}{[\cosh\psi-\cos(\phi-\phi')]^q}. \tag{A3}$$

The obvious change of variables $\phi = \phi_1+\phi_2$, $\phi' = \phi_1-\phi_2$ reduces $I^{p,q}_{m,m'}$ to the product of an elementary integral times a second integral which, for the small values of p and q required, is straightforwardly, if somewhat tediously, evaluated by the same contour method as (A2). The case $(m,m',p,q) = (0,0,2,2)$ leads to (2.18), while $(m,m',p,q) = (0,0,4,3)$ leads to (2.19).

To derive (2.20) one needs to calculate the matrix elements required, $U^{(1)}_{m,0}$, since this term is the usual sum over states of squared matrix elements divided by energy denominators. These matrix elements involve the integral $I^{2,2}_{m,0}$. It follows from the elementary integration alluded to in the above paragraph that this integral is nonvanishing only for $m = \pm 2$. Thus, only $I^{2,2}_{2,0}$ is needed. As mentioned in the body of the paper, s-wave pairing couples only to d-wave pairing at this order. The single zeroth-order energy denominator in the standard second-order perturbation theory formula is then given in terms of the zeroth-order matrix elements (2.16). Putting together these pieces one obtains (2.20).

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