Possible large relative enhancement of the superconducting T_c by anisotropy

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The enhancement of the superconducting transition temperature T_c by anisotropy is studied as a function of the Coulomb repulsion μ^*. Numerical solutions of the anisotropic Eliashberg equations are presented with isotropic μ^* ranging up to and beyond the average electron-phonon parameter λ, assuming separable anisotropy. An approximate anisotropic T_c equation is developed, tested against the numerical results, and used to interpret them. It is found that the dependence of μ^* on the upper phonon cutoff plays an important role. Further, within BCS-like approximations, a general formalism is developed applicable to any anisotropy function. It is applied, in connection with calculated microscopic parameters in real metals, to develop additional insight into the role played by μ^* in criteria for superconductivity.

I. INTRODUCTION

The enhancement of the superconducting transition temperature T_c due to anisotropy in the effective electron-electron interaction has been treated theoretically in a number of models, most of which require that the anisotropy is small, in a sense discussed below. The primary, although not sole, focus of this paper is a further discussion of the regime in which the relative enhancement can be very large, even for modest anisotropy. Most of this introduction consists of a brief discussion of related earlier work, through which a number of quantities used later are introduced.

The part of the theory introduced by Markowitz and Kadanoff[1] for pure crystals (which are all that are treated here) is a generalization of the original BCS theory[2] to include anisotropy in the pairing interaction $V_{\vec{k}\vec{k}'}$, in a simple way, namely the separable model. The resulting T_c equation differs from the BCS one only in that the average interaction V is multiplied by the factor $1+\langle a^2\rangle$, where $\langle a^2\rangle$ is the mean-square anisotropy of both $V_{\vec{k}\vec{k}'}$ and, in this model, the energy gap. The enhancement of T_c relative to its corresponding isotropic value T_c^i is [$N(0)$ is the electron density of states at the Fermi energy]

$$\frac{T_c}{T_c^i}=e^{\langle a^2\rangle/N(0)V}, \tag{1}$$

which can be expanded to $1+\langle a^2\rangle/N(0)V$ if the argument of the exponential is small. This enhancement is generally of order 20% or less for $\langle a^2\rangle \lesssim 0.04$. This model unambiguously implies the same criterion for superconductivity as does the isotropic BCS theory, namely that the average interaction must be attractive; in this formalism, $V>0$.

Numerical solutions of the anisotropic Eliashberg equations have also been obtained.[3-5] In this case the underlying anisotropic quantity is $[\alpha^2F(\omega)]_{\vec{k}\vec{k}'}$, which is the electron-phonon spectral function for scattering of an electron from $\vec{k}$ to $\vec{k}'$ on the Fermi surface due to a phonon of energy ω. Again using $\langle a^2\rangle \lesssim 0.04$, the enhancement of T_c was on the order of 10% for most specific materials considered, although for a weak coupling case such as Al it can reach $\sim 30\%$ because of the smaller value of λ, the average electron-phonon mass-enhancement parameter.

In these treatments, the changes in T_c are often evaluated only to $O(\langle a^2\rangle)$. This requires that $\langle a^2\rangle$ be small in the sense that

$$\frac{\langle a^2\rangle}{\lambda-\mu^*(\omega_{co})} \ll 1 , \tag{2}$$

or in the BCS-like theory, $\langle a^2\rangle/N(0)V \ll 1$. In Eq. (2), $\mu^*(\omega_{co})$ is the Coulomb parameter used in solving the Eliashberg equations which depends on the cutoff frequency ω_{co}, as will be discussed in the next section. In the same spirit as Markowitz and Kadanoff, Whitmore and Carbotte[6] introduced a simple model to investigate qualitatively the regime in which condition (2) does not hold. Because the attractive part of $V_{\vec{k}\vec{k}'}$ is presumably dominated by the anisotropic electron-phonon interaction ($V_{e\text{-ph}}$) and the repulsive part by a less anisotropic Coulomb interaction (V_C), a BCS-like theory was developed with

$$V_{\vec{k}\vec{k}'}=(1+a_{\vec{k}})V_{e\text{-ph}}(1+a_{\vec{k}'})-V_C . \tag{3}$$

Both $V_{e\text{-ph}}$ and V_C are positive, and the Fermi-surface average of $a_{\vec{k}}$ is zero, as in all separable models. In the

original treatment, both parts of the interaction were truncated at the maximum phonon energy ω_m, and μ^* was identified with $N(0)V_C$. This is easily modified to allow the Coulomb interaction to extend up to the Fermi energy ϵ_F, as for the isotropic case.[7-9] The T_c equations, given in the Appendix [(A8), (A13), and (A14)], are the same as in Ref. 6, but with μ^* clearly given by

$$\mu^*(\omega_m)=\frac{N(0)V_C}{1+N(0)V_C\ln(\epsilon_F/\omega_m)} . \tag{4}$$

In the regime of small $\langle a^2\rangle$ [satisfying (2)], this model gives[10]

$$T_c/T_c^i\simeq 1+\langle\alpha^2\rangle , \tag{5}$$

where $\langle\alpha^2\rangle$ is the mean-square energy gap, which in this case is just $\langle a^2\rangle/[1-\mu^*/N(0)V_{e\text{-ph}}]$. Thus this is essentially the same as Eq. (1) if the latter is interpreted as referring to the gap anisotropy. However, when (2) does not hold, i.e., when $\mu^*(\omega_m)$ approaches $N(0)V_{e\text{-ph}}$, then the relative enhancement of T_c can become very large. In fact when it equals or even exceeds $N(0)V_{e\text{-ph}}$, T_c^i vanishes, but superconductivity can persist (in this model) because of the anisotropy.

None of these results were meant to be interpreted quantitively, primarily because of the use of BCS-type approximations and the assumption of separable anisotropy. Leavens *et al.*[11] have emphasized both these points. They found that using nonseparable anisotropy could either increase or decrease the enhancement within a BCS-like model. However, for any form of the anisotropy, a finite T_c persists for some $\mu^*(\omega_m)>\lambda$.

The rest of this paper focuses primarily on the regime of large $\mu^*(\omega_{co})$, by which is meant that $\mu^*(\omega_{co})$ is sufficiently large that most previous work would imply that superconductivity would not stabilize at any temperature. In addition to specific numerical results, one would ideally like to derive a "clean" statement of necessary and sufficient conditions for the Eliashberg equations to have a finite-T_c solution, or alternatively to determine T_c numerically as a function of $\mu^*(\omega_{co})$ for all $\mu^*(\omega_{co})$ until T_c vanishes. Unfortunately the first alternative has remained elusive, and the second is not feasible because as $\mu^*(\omega_{co})$ increases, T_c decreases, causing a very large increase in the required computing resources. Consequently, no clear criteria have been established.

Nevertheless, two somewhat different approaches have been pursued, leading to perhaps surprising results. The first, described in Sec. II, consists of both numerical and approximate solutions of the anisotropic Eliashberg equations with separable anisotropy. Solutions are given for $\mu^*(\omega_{co})$ much larger than the value for which, for example, the McMillan equation would predict a finite T_c to be possible, and indeed for $\mu^*(\omega_{co})>\lambda$ for any cutoff frequency greater than $3\omega_m$. Complementing this, Sec. III deals with nonseparable realistic anisotropy functions but only within a BCS-like approximation. It is found that general statements about the existence or nonexistence of a finite T_c, which depend on the details of the anisotropy in the attractive part of the pairing potential, can be formulated. Specific examples are considered. In Sec. IV, conclusions are drawn.

II. ELIASHBERG THEORY WITH SEPARABLE ANISOTROPY

The main result of this section is the numerical solution of the anisotropic Eliashberg equations for T_c as a function of $\mu^*(\omega_{co})$, which is varied up to and beyond λ. These equations, written on the imaginary-frequency axis, are[12-14]

$$\tilde{\Delta}_{\vec{k}}(p)=\pi T_c\sum_q\left\langle[\lambda_{\vec{k}\,\vec{k}'}(p-q)-\mu^*(\omega_{co})]\frac{\tilde{\Delta}_{\vec{k}'}(q)}{|\tilde{\omega}_{\vec{k}'}(q)|}\right\rangle' \tag{6}$$

and

$$\tilde{\omega}_{\vec{k}}(p)=\omega_p+\pi T_c\sum_q\langle\lambda_{\vec{k}\,\vec{k}'}(p-q)\rangle'\mathrm{sgn}(\omega_q) , \tag{7}$$

with

$$\lambda_{\vec{k}\,\vec{k}'}(p-q)=2\int_0^{\omega_m}\frac{d\omega}{\omega^2+(\omega_p-\omega_q)^2}[\alpha^2F(\omega)]_{\vec{k}\,\vec{k}'} . \tag{8}$$

The ω_p are Matsubara frequencies, $i\omega_p=i\pi T_c(2p-1)$, and λ is the double average, $\lambda=\langle\langle\lambda_{\vec{k}\,\vec{k}'}(0)\rangle'\rangle$. The sums in Eqs. (6) and (7) are truncated at $N_c=(\omega_{co}/\pi T_c+1)/2$, where ω_{co} is usually some integral multiple of ω_m. From Eq. (4) one easily finds that for two different cutoffs, ω_{co} and ω'_{co}, the corresponding Coulomb parameters are related through

$$\mu^*(\omega'_{co})=\frac{\mu^*(\omega_{co})}{1+\mu^*(\omega_{co})\ln(\omega_{co}/\omega'_{co})} . \tag{9}$$

The cutoff frequency needs to be large enough that the phonon contribution to the sums converges. In practice, numerical tests using an $\alpha^2F(\omega)$ similar to that of Ga indicated that as long as $\omega_{co}\geq 3\omega_m$, T_c was insensitive to ω_{co} to within about 2%, provided that $\mu^*(\omega_{co})$ was rescaled according to (9). Thus the Coulomb parameter is a well-defined, albeit a complicated, function of the material parameters and of ω_{co}. It is essential to keep in mind its dependence on ω_{co}.

For a given cutoff, Eq. (4) also implies an upper limit on $\mu^*(\omega_{co})$, namely $1/\ln(\epsilon_F/\omega_{co})$, even if $N(0)V_C$ were to become very large. For typical values of ϵ_F and ω_{co}, this is on the order of 0.3 or 0.4 for cutoffs of $3\omega_m$, or the more commonly used $10\omega_m$, respectively. (The effective value could be larger, for example, because of paramagnons,[15,16] but probably not by a large amount.)

Computationally, the largest $\mu^*(\omega_{co})$ which can be treated is limited by the fact that as it approaches λ, T_c decreases by orders of magnitude, so that N_c increases by orders of magnitude. To investigate this regime, solutions have been obtained using the separable-anisotropy model, the spectral density $\alpha^2F(\omega)$ calculated for Al by Leung *et al.*,[17] and a cutoff frequency of $\omega_{co}=3\omega_m$. In order to keep T_c reasonable, unrealistically large values of $\langle a^2\rangle$ had to be used, namely 0.09 and 0.16, but we do not believe this to be significant. To this $\alpha^2F(\omega)$ corresponds a value $\lambda=0.436$, and therefore an increase of $\mu^*(3\omega_m)$ just beyond this λ is near to the limit of physically reasonable values, barring the effects of paramagnons or other processes. Thus these choices of $\alpha^2F(\omega)$ and $\langle a^2\rangle$ provide a computationally accessible region, which is still within the

limits of physically acceptable values of $\mu^*(3\omega_m)$. There is nothing in the calculations (or the later analysis) to suggest that the results could be qualitatively different for smaller values of λ or $\langle a^2\rangle$. The main point is the existence of nontrivial solutions in this regime, and in particular the very large relative enhancement of T_c, as compared with the case of $\mu^*(\omega_{co}) \ll \lambda$.

With a separable model used for $[\alpha^2F(\omega)]_{\vec{k}\vec{k}'}$, Eqs. (6) and (7) can be set in the form of ordinary isotropic Eliashberg equations which can be solved numerically in a now standard way. It is easily seen that the solution of Eq. (6) has the form $\tilde{\Delta}_{\vec{k}}(p)=\tilde{\Delta}_0(p)+a_{\vec{k}}\tilde{\Delta}_1(p)$, with

$$\tilde{\Delta}_1(p)=\pi T_c \sum_q \lambda(p-q)[(r_q+s_q)\tilde{\Delta}_0(q) + (s_q+t_q)\tilde{\Delta}_1(q)] \tag{10}$$

and

$$\tilde{\Delta}_0(p)=\tilde{\Delta}_1(p)-\mu^*(\omega_{co})M\ , \tag{11}$$

with

$$M=\pi T_c \sum_q [r_q\tilde{\Delta}_0(q)+s_q\tilde{\Delta}_1(q)] \tag{12}$$

and

$$r_p=\left\langle \frac{1}{|\tilde{\omega}_{\vec{k}}(p)|}\right\rangle,\quad s_p=\left\langle \frac{a_{\vec{k}}}{|\tilde{\omega}_{\vec{k}}(p)|}\right\rangle, \tag{13}$$

$$t_p=\left\langle \frac{a^2_{\vec{k}}}{|\tilde{\omega}_{\vec{k}}(p)|}\right\rangle .$$

In Eq. (10), $\lambda(p-q)$ is given by (8) using the isotropic spectral density $\alpha^2F(\omega)$. After some simple algebra an equation for $\tilde{\Delta}_0(p)$ is obtained from (10)–(12),

$$\tilde{\Delta}_0(p)=\pi T_c \sum_q [\lambda(p-q)(r_q+2s_q+t_q) - \mu_p^*(r_q+s_q)]\tilde{\Delta}_0(q)\ , \tag{14}$$

$$\mu_p^*=\mu^*(\omega_{co})\frac{1-\pi T_c\sum_q \lambda(p-q)(s_q+t_q)}{1-\mu^*(\omega_{co})\pi T_c\sum_q s_q}\ . \tag{15}$$

Solutions of these equations are exhibited in Fig. 1 (——). The first thing to notice is that T_c remains finite and well behaved up to and beyond the point $\mu^*(3\omega_m)=\lambda$, a result consistent with the original BCS-like results of Whitmore and Carbotte.

In order to compare the results with the corresponding isotropic limit, an approximate T_c equation is derived which is a generalization of an equation of Leavens and Carbotte.[18] This is done in Appendix A. As one would expect, the enhancement of T_c by anisotropy is quite modest as long as $\mu^*(3\omega_m)$ is small; the enhancement is given approximately by

$$\frac{T_c}{T_c^i}\simeq\exp\left[\frac{(1+\lambda)\langle\alpha^2\rangle}{\lambda-\mu^*(\omega_m)}\right]. \tag{16}$$

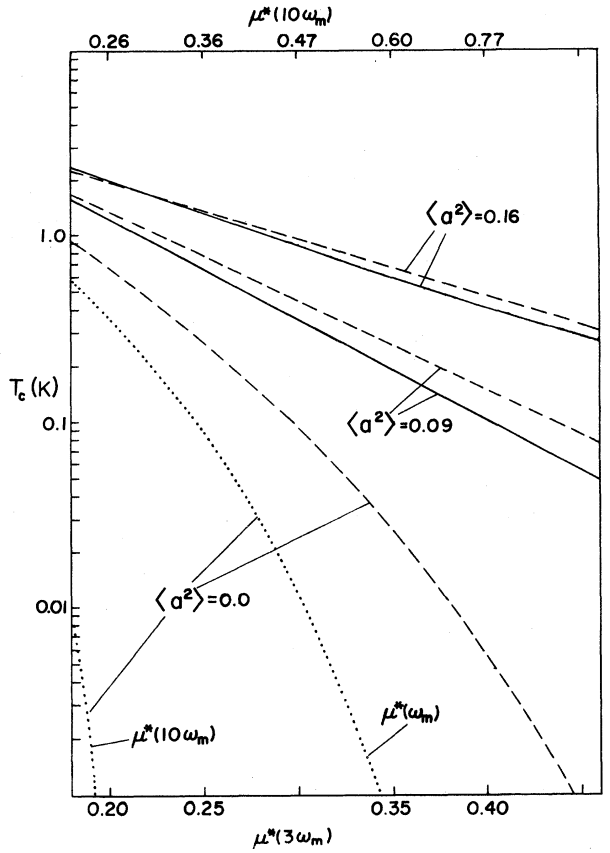

FIG. 1. Comparison of approximate T_c expressions with the full solutions of the Eliashberg equations, for the isotropic and separable anisotropic limits. The solid curves are the full calculations (——), the dashed curves the Leavens-Carbotte–type equation generalized to include the anisotropy, Eqs. (A8)–(A10) of this paper (— — —), and the dotted curves result from the McMillan equation (· · ·). The lower curve uses $\mu^*(10\omega_m)$, and the upper curve uses $\mu^*(\omega_m)$. Using a value $\mu^*(3\omega_m)$ would result in a curve between these two.

$\langle\alpha^2\rangle$ is again the mean-square gap anisotropy, shown by Carbotte and Daams[19] to be

$$\langle\alpha^2\rangle=\left[\frac{\lambda(1+\mu^*(\omega_m))+\bar{\lambda}\mu^*(\omega_m)}{(1+\lambda)[\lambda-\mu^*(\omega_m)]}\right]^2\langle a^2\rangle \tag{17}$$

within this model and in this limit. However, for all the curves shown in Fig. 1, Eqs. (16) and (17) are inadequate approximations to Eqs. (A8)–(A10), which include the anisotropy to all orders. Using those equations it is found that at $\mu^*(3\omega_m)=\lambda$, the relative enhancement is on the order of 2 orders of magnitude; for smaller anisotropy, qualitatively the same results can be expected. As $\mu^*(3\omega_m)$ is further increased, the relative enhancement becomes much larger; if it were large enough that $\mu^*(\omega_m)$ also equaled or even exceeded λ (as could certainly be the case for a smaller λ than that used in the calculations), T_c is predicted to remain finite in this model, as long as $\langle a^2\rangle>0$. Note, however, that the regime $\mu^*(\omega_m)\simeq\lambda$ has not been treated in the *numerical* solution of the Eliashberg equations.

That the *isotropic* T_c^i remains finite for $\mu^*(3\omega_m)>\lambda$ may be surprising. It is even more surprising when it is recalled that for any cutoff ω_{co} larger than $3\omega_m$, $\mu^*(\omega_{co})$ becomes larger than $\mu^*(3\omega_m)$. For instance, at $\mu^*(3\omega_m)=0.46$, $\mu^*(10\omega_m)$ is equal to $1.03\simeq 2.4\lambda$, as is easily verified by use of Eq. (9). [The $\mu^*(10\omega_m)$ scale is included in Fig. 1.] It is critical that what appears in Eq. (16) is $\mu^*(\omega_m)$, which in fact does not exceed the value of 0.3, and which therefore is still smaller than λ.

The prediction of a finite T_c^i is in sharp contrast with other approximate T_c formulas,[20–22] at least as they are conventionally used. The McMillan equation, for example, predicts T_c^i to vanish at $\mu^*(\omega_{co})=\lambda/(1+0.62\lambda)$. Although the cutoff is not precisely specified, it is generally taken to be $10\omega_m$. This then corresponds to T_c^i vanishing at $\mu^*(3\omega_m)=0.24$, much less than λ. From Fig. 1 it is clear that the McMillan equation with such a high cutoff in μ^* grossly underestimates T_c^i throughout this range.

The use of $\mu^*(\omega_m)$ somewhat improves the agreement. A careful examination of McMillan's derivation indicates that the appropriate cutoff to be used in μ^* is the Debye energy divided by 1.4. For small μ^* (or large λ), this distinction is not important and generally one uses the tunneling value [probably $\mu^*(10\omega_m)$] or simply 0.1 or 0.13. However, as seen from the figure, even if the μ^* appropriate to a cutoff of ω_m is used, the McMillan equation still grossly underestimates T_c. The dependence of T_c on the choice of cutoff has not been emphasized previously in the literature.

To summarize so far, numerical solutions for separable anisotropy have been exhibited in the range $0.18\leq\mu^*(3\omega_m)\leq 1.05\lambda$. Furthermore, since $\mu^*(\omega_{co})$ is an increasing function of ω_{co}, for any acceptable cutoff used the corresponding $\mu^*(\omega_{co})$ is even larger. The approximate formula presented appears to be at least qualitatively correct throughout the range of $\mu^*(\omega_{co})$, which, for this spectrum at least, is in contrast to the McMillan equation.

Because of the dependence of $\mu^*(\omega_{co})$ on ω_{co}, one is also led to the conclusion that within Eliashberg theory, even for the isotropic case, no particular significance can be attached to the point $\mu^*(\omega_{co})=\lambda$, because one could change ω_{co}, and hence $\mu^*(\omega_{co})$ in a perfectly acceptable way.

As a final point, it is noted that the approximate T_c formula derived here for separable anisotropy predicts that arbitrarily large $\mu^*(\omega_m)$ could be tolerated as long as there is some anisotropy. As a further generalization of the T_c equation used here, the following model anisotropy has been examined:

$$[\alpha^2F(\omega)]_{\vec{k}\vec{k}'}=\alpha^2F(\omega)(1+a_{\vec{k}}+a_{\vec{k}'}+\gamma a_{\vec{k}}a_{\vec{k}'}), \qquad (18)$$

for which the separable model is recovered when $\gamma=1$. For a certain range of γ, a finite $\mu^*(\omega_m)$ can drive T_c to zero, but for any γ, a finite T_c persists for some $\mu^*(\omega_m)>\lambda$. In fact, in the most detrimental case for T_c considered by Leavens *et al.*,[11] which corresponds to negative γ, the condition on μ^* to have a solution is $\mu^*<[(1+|\gamma|)/|\gamma|]\lambda$. This condition makes no reference to the size of the anisotropy but only to the nonseparability coefficient. The model (18) is not perfectly general, but was used by Leavens *et al.*[11]

III. BCS THEORY WITH NONSEPARABLE ANISOTROPY

In contrast to the approach of the preceding section, within the BCS approximation, nonseparable anisotropy can be explored in a general way. Although nonquantitative, such a model at least produced the same qualitative behavior in the new regime [with $N(0)V_{e\text{-ph}}$ identified as λ] for both the isotropic and separable anisotropic cases, as did the Leavens-Carbotte–type approximations. This is in marked contrast with other approximate expressions which predict T_c to vanish for much smaller values of $\mu^*(\omega_m)$.

Two different cases are considered. The first is a general analysis which will be used in conjunction with numerical calculations of $\lambda_{\vec{k}\vec{k}'}$ in Pb (Ref. 3) and Al;[4] the second is more specific and is used with numerical calculations in the alkali metals.[23]

Within the BCS approximations, the T_c equation reduces to

$$\tilde{\Delta}_{\vec{k}}=\pi T_c\sum_p{}'\left\langle[\lambda_{\vec{k}\vec{k}'}-\mu^*(\omega_m)]\frac{\tilde{\Delta}_{\vec{k}'}}{|\omega_p|}\right\rangle', \qquad (19)$$

with the sums truncated at ω_m. The major approximation of (19) is the ignoring of the anisotropic mass renormalization in $\omega_{\vec{k}}(p)$, Eq. (7), which can be approximated by $\omega_{\vec{k}}(p)\simeq[1+\lambda(1+a_{\vec{k}})]\omega_p$. The isotropic part of this term can easily be incorporated by multiplying the eigenvalue f introduced in Eq. (26) which follows by $1+\lambda$, which would have a large quantitative effect on the formula for T_c, but which would not alter the qualitative behavior, in particular, the conditions for a finite T_c. The anisotropic renormalization cannot, unfortunately, be incorporated into the present formalism.

For the general treatment of anisotropy, it is convenient to work in terms of the Fermi-surface harmonics (FSH's) introduced by Allen,[24] which are a set of functions $\psi_l(\vec{v}_{\vec{k}})$ which are orthonormal over the Fermi surface of interest. The Fermi surface can consist of N distinct pieces, and a particular ψ_l is nonzero on only one of them, denoted $i(l)$. The order of ψ_l is denoted $O(l)$. The relative weights of different regions are related to the partial and complete densities of states through

$$W_{i(l)}=\int_{i(l)}\frac{dS_{\vec{k}}}{|v_{\vec{k}}|}\Big/\int\frac{dS_{\vec{k}}}{|v_{\vec{k}}|}, \qquad (20)$$

where the integral in the numerator of (20) is over the surface $i(l)$, whereas that in the denominator is over the entire Fermi surface. The orthonormality of the ψ_l is expressed through the inner product

$$\langle\psi_l|\psi_{l'}\rangle\equiv\int\frac{dS_{\vec{k}}}{|v_{\vec{k}}|}\psi_l(\vec{v}_{\vec{k}})\psi_{l'}(\vec{v}_{\vec{k}})\Big/\int\frac{dS_{\vec{k}}}{|v_{\vec{k}}|}$$

$$=\delta_{ll'}. \qquad (21)$$

These are used for expansions

$$\Delta_{\vec{k}}=\sum_l \Delta_l \psi_l(\vec{v}_{\vec{k}}) , \tag{22}$$

$$\begin{Bmatrix} \lambda_{\vec{k}\vec{k}'} \\ \mu^*(\omega_m) \end{Bmatrix} = \sum_{l,l'} \begin{Bmatrix} \lambda_{ll'} \\ \mu^*_{ll'} \end{Bmatrix} \psi_l(\vec{v}_{\vec{k}})\psi_{l'}(\vec{v}_{\vec{k}'}) , \tag{23}$$

with coefficients given by

$$\Delta_l = \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|}\psi_l(\vec{v}_{\vec{k}})\Delta_{\vec{k}} \Big/ \int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} , \tag{24}$$

$$\begin{Bmatrix} \lambda_{ll'} \\ \mu^*_{ll'} \end{Bmatrix} = \frac{\displaystyle\int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} \int \frac{dS_{\vec{k}'}}{|v_{\vec{k}'}|}\psi_l(\vec{v}_{\vec{k}})\psi_{l'}(\vec{v}_{\vec{k}'}) \begin{Bmatrix} \lambda_{\vec{k}\vec{k}'} \\ \mu^*(\omega_m) \end{Bmatrix}}{\displaystyle\int \frac{dS_{\vec{k}}}{|\vec{v}_{\vec{k}}|} \int \frac{dS_{\vec{k}'}}{|\vec{v}_{\vec{k}'}|}} . \tag{25}$$

Substituting these into Eq. (19) leads to the following eigenvalue equation:

$$\frac{1}{f}\Delta_l = \sum_{l'} \kappa_{ll'}\Delta_{l'} , \tag{26}$$

with kernel

$$\kappa_{ll'}=\lambda_{ll'}-\mu^*_{ll'} . \tag{27}$$

T_c is determined by the largest eigenvalue, say f_1; if $f_1>0$, then $f_1=\ln(1.13\omega_m/T_c)$, as usual. Thus once the expansion coefficients are known, the calculation reduces to finding f_1.

From the normalization, the zeroth-order functions are

$$\psi^0_l(\vec{v}_{\vec{k}}) = \begin{cases} 1/(W_{i(l)})^{1/2} & \text{for } \vec{k}\in i(l), \\ 0 & \text{otherwise,} \end{cases} \tag{28}$$

and the coefficients of the (assumed constant) $\mu^*(\omega_m)$ are

$$\mu^*_{ll'} = \begin{cases} \mu^*(\omega_m)(W_{i(l)}W_{i(l')})^{1/2} & \text{for } O(l)=O(l')=0, \\ 0 & \text{otherwise.} \end{cases} \tag{29}$$

For a Fermi surface with N distinct pieces, $\mu^*_{ll'}$ is an $N\times N$ matrix, but with rank of only 1.

In passing, it is noted that for a separable model, the kernel, $\underline{\kappa}$, has the form

$$\kappa_{ll'}=\lambda\alpha_l\alpha_{l'}-\mu^*_{ll'} , \tag{30}$$

where the α_l are the expansion coefficients of $(1+a_{\vec{k}})$.

The results of two earlier calculations are used; the first is that for Pb by Daams,[3] and the second is for Al by Daams and Carbotte.[4] In each case it was found that $\lambda_{\vec{k}\vec{k}'}$ is almost "sheet constant," i.e., that as $\vec{k}$ or $\vec{k}'$ varies within any of the four separate sheets of the Fermi surface, there is little variation in $\lambda_{\vec{k}\vec{k}'}$, but when either switches to another sheet, there is a larger change. As a consequence, the expansion is dominated by the four zeroth-order FSH's. The calculations are summarized in Tables I and II. In interpreting these tables it is worth noting that for $\vec{k}\in i(l)$, $\vec{k}'\in i(l')$, then to the lowest order,

$$\lambda_{\vec{k}\vec{k}'}\simeq\lambda_{ll'}\psi^0_l(\vec{v}_{\vec{k}})\psi^0_{l'}(\vec{v}_{\vec{k}'})=\frac{\lambda_{ll'}}{(W_{i(l)}W_{i(l')})^{1/2}} . \tag{31}$$

T_c was calculated as a function of $\mu^*(\omega_m)$ for each of these, with the $\lambda_{ll'}$ truncated to retain only the leading 4×4 submatrices; the results are illustrated in Fig. 2 (— — —). To compare with the separable model, for each set of data $\langle a^2\rangle$ was found and used in the early expression of Whitmore and Carbotte, Eqs. (A8), (A13), and (A14); the results are also shown in the figure by solid lines. The dotted lines are the results for the corresponding isotropic limit.

Two general comments can be made. First, in both the separable and nonseparable models, the modest anisotropy in $\lambda_{\vec{k}\vec{k}'}$ leads to a very large relative enhancement of T_c as $\mu^*(\omega_m)$ increases, diverging as $\mu^*(\omega_m)$ surpasses λ with no qualitative differences between the two. Second, the separable model exaggerates the enhancement for these $\lambda_{\vec{k}\vec{k}'}$.

Particularly in view of the comments of Leavens *et al.*[11] it is interesting to ask whether or not a large $\mu^*(\omega_m)$ could suppress superconductivity altogether. Within the BCS approximations, a necessary and sufficient condition for a

TABLE I. Zeroth-order anisotropy calculations for Pb by Daams (Ref. 3). The double–Fermi-surface average of $\lambda_{\vec{k}\vec{k}'}$ is $\lambda=1.33$, and the mean-square anisotropy in $\lambda_{\vec{k}\vec{k}'}$ is $\langle a^2\rangle=0.035$.

Regions				
$i(l)$	$i(l')$	$W_{i(l)}W_{i(l')}$	$\lambda_{ll'}/\lambda$	$\mu^*(\omega_m)_{ll'}/\mu^*(\omega_m)$
1	1	0.001	0.0083	0.032
1	2	0.014	0.111	0.118
1	3	0.009	0.100	0.095
1	4	0.004	0.062	0.063
2	2	0.258	0.577	0.508
2	3	0.167	0.393	0.409
2	4	0.069	0.316	0.263
3	3	0.108	0.179	0.329
3	4	0.044	0.213	0.210
4	4	0.018	0.175	0.134

TABLE II. Zeroth-order anisotropy calculations for Al by Daams and Carbotte (Ref. 4) using the notation of Table I, $\lambda=0.439$ and $\langle a^2\rangle=0.011$.

Regions $i(l)$	$i(l')$	$W_{i(l)}W_{i(l')}$	$\lambda_{ll'}/\lambda$	$\mu^*(\omega_m)_{ll'}/\mu^*(\omega_m)$
1	1	0.332	0.619	0.576
1	2	0.079	0.268	0.282
1	3	0.087	0.330	0.295
1	4	0.078	0.242	0.279
2	2	0.019	0.117	0.138
2	3	0.021	0.143	0.144
2	4	0.019	0.105	0.137
3	3	0.023	0.175	0.151
3	4	0.020	0.129	0.143
4	4	0.018	0.094	0.135

finite T_c is that the real symmetric matrix κ has at least one positive eigenvalue. This can be investigated using the theorem discussed in Appendix B, which can be summarized as follows.

(1) For a particular value of $\mu^*(\omega_m)$,

(a) if any diagonal element κ_{ll} is positive, or

(b) if any leading principal minor M_n satisfies

$$\mathrm{sgn}(M_n)=(-1)^n\ ,$$

then there is at least one positive eigenvalue.

(2) If the matrix $\underline{\Lambda}=\{\lambda_{ll'}\}$ has two positive eigenvalues, then superconductivity occurs for arbitrarily large $\mu^*(\omega_m)$ (as in the separable model).

Condition (1) suggests that rather restrictive conditions are necessary to prevent a real materials exhibiting superconductivity at some temperature, particularly since an isotropic Coulomb repulsion contributes only to those elements of $\mu^*_{ll'}$ for which $O(l)=O(l')=0$. (This assumes no other critical mechanism such as, perhaps, paramagnons.) Condition (2) implies that the coefficients $\lambda_{ll'}$ alone determine whether an arbitrarily large $\mu^*(\omega_m)$ can be tolerated.

Returning to the numerical calculations, it is easy to establish that each of the two matrices whose first 16 elements are the $\lambda_{ll'}$ listed in the tables has at least two positive eigenvalues, *independent* of what the rest of the elements are (for example, by the method of Lagrange reduction[24]). Thus, just as for separable anisotropy, an infinite $\mu^*(\omega_m)$ would not drive T_c to zero. Note also that even though the magnitude of T_c depends very sensitively on the average λ, this existence of a finite T_c does not, but rather depends only on the anisotropy in $\lambda_{\vec{k}\vec{k}'}$.

In the second part of this section, anisotropy in the alkali metals Na, K, and Rb is considered. Plane-wave electron states and a spherical Fermi surface are assumed, so that spherical harmonics are the appropriate basis functions, labeled by the set of indices (l,m); the expansions are modified slightly because the Y_l^m are complex. The anisotropy enters via the phonons and umklapp processes.

Within these approximations, the eigenvalue equation becomes

$$\frac{1}{f}\Delta_{lm}=\sum_{l'm'}\kappa_{lml'm'}\Delta_{l'm'}\ , \tag{32}$$

with

$$\kappa_{lml'm'}=\frac{\lambda_{lml'm'}}{4\pi}-\mu^*(\omega_m)\delta_{l0}\delta_{l'0}\delta_{m0}\delta_{m'0} \tag{33}$$

and

$$\lambda_{lml'm'}=\int d\Omega_{\vec{k}}\int d\Omega_{\vec{k}'}Y_l^m(\Omega_{\vec{k}})^*Y_{l'}^{m'}(\Omega_{\vec{k}'})\lambda_{\vec{k}\vec{k}'}\ . \tag{34}$$

The first theorem of Appendix B implies that a suffi-

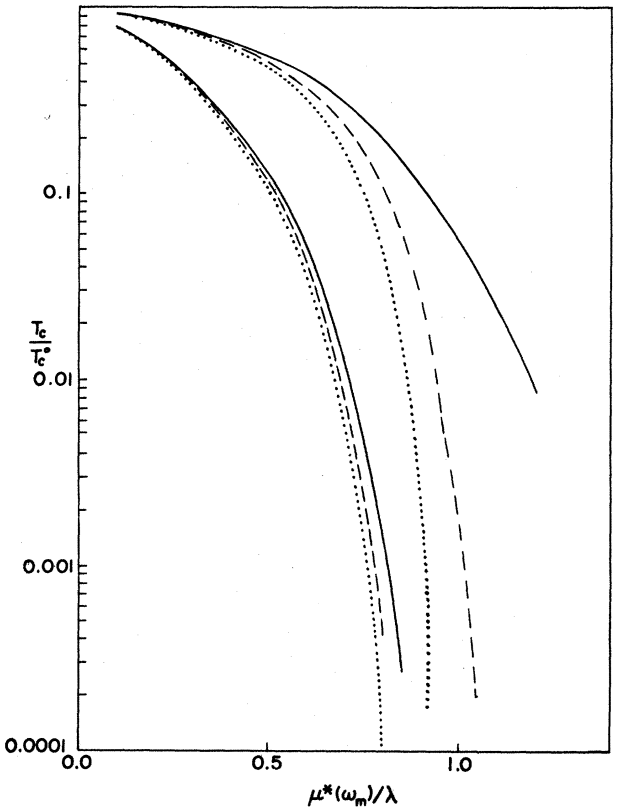

FIG. 2. Reduction in T_c with increasing $\mu^*(\omega_m)$ for the calculated anisotropic $\lambda_{\vec{k}\vec{k}'}$ of Pb (upper curves) and Al (lower curves) in a BCS-like theory. T_c^0 is the transition temperature found from the eigenvalue problem with $\mu^*(\omega_m)=0$. The solid curves are for the corresponding separable model (——), the dashed curves are obtained from the $\lambda_{ll'}$ matrices (— — —), and the dotted curves are for the corresponding isotropic limits (· · ·). At $\mu^*(\omega_m)$ the separable model T_c agrees with the eigenvalue problem T_c to about 1%.

cient condition for a finite T_c is that at least one diagonal element of $\underline{\kappa}$ be positive. Since $\lambda_{0000}=4\pi\lambda$, the first condition is that $\lambda>\mu^*(\omega_m)$, as for the isotropic model. If this is not satisfied, then it would suffice for some other diagonal element λ_{lmlm} to be positive, since for $l\geq 1$, the $\mu^*(\omega_m)$ does not appear.

Leavens and Carbotte[23] have calculated related quantities for Na, K, and Rb using fitted force-constant models for the phonons and a variety of pseudopotentials. What is of direct interest here is the $g_l^{e\text{-ph}}$ which are related via

$$g_l^{e\text{-ph}}=\frac{1}{4\pi(2l+1)(1+\lambda)}\sum_{m=-l}^{l}\lambda_{lmlm}\ . \tag{35}$$

In particular, they found that in all cases, $g_1^{e\text{-ph}}>0$, so that $\lambda_{1m1m}>0$ for at least one value of m. Hence even if $\mu^*(\omega_m)>\lambda$, as long as it is taken to be isotropic, $\underline{\kappa}$ has at least one positive eigenvalue, implying a finite although presumably very small T_c.

In ending this section it is stressed again that the formalism ignores the anisotropy in the mass renormalization of the $\tilde{\omega}_{\vec{k}}(p)$ although the conclusions are independent of the isotropic part, $1+\lambda$. Because this regime of large $\mu^*(\omega_m)$ depends sensitively on the anisotropy, it would certainly be desirable to extend this type of analysis to include this additional complication.

IV. SUMMARY

The main focus of this paper has been the regime of large $\mu^*(\omega_{co})$, in the sense that it is large enough to violate the condition $\langle a^2\rangle/[\lambda-\mu^*(\omega_{co})]\ll 1$, or in that most previous treatments of T_c imply that superconductivity would not exist at any finite temperature.

The major calculations presented are numerical solutions of the Eliashberg T_c equations, assuming isotropic μ^* and *separable* anisotropy in $l_{\vec{k}\vec{k}'}$, into the range $\mu^*(3\omega_m)>\lambda$. It was pointed out that a larger cutoff frequency would require an even larger μ^*, but should not affect the results. Comparison with the isotropic limit, through the generalization of a very useful approximate T_c equation, showed a very large relative enhancement of T_c by the anisotropy in this regime, particularly relative to the usual regime of $\langle a^2\rangle/[\lambda-\mu^*(\omega_{co})]\ll 1$. The result that T_c persists for some $\mu^*(\omega_m)>\lambda$ even for nonseparable anisotropy, within this approximate equation, was also found.

Results using the McMillan equation were also compared, and at least for this case, found to be far too small when as is conventional $\mu^*(10\omega_m)$ is used; this was attributed to the term $\mu^*(10\omega_m)(1+0.62\lambda)$ appearing in the denominator of the exponential. This suggested an examination of the dependence of $\mu^*(\omega_{co})$ on the cutoff ω_{co}, and the realization that the statement $\mu^*>\lambda$ is not well defined, and therefore not likely to provide a criterion for superconductivity. This is also consistent with numerical solutions of the isotropic Eliashberg equations using very large cutoffs.[26]

Within a BCS-like approach, anisotropy was examined in a more general way. Although for certain models of anisotropy, a finite $\mu^*(\omega_m)$ can destroy superconductivity, for the two anisotropy functions for which detailed numerical results are available, an arbitrarily large $\mu^*(\omega_m)$ could in fact be tolerated. Finally, a simple analysis of numerical calculations in Na, K, and Rb suggested that even in the alkali metals anisotropy may induce superconductivity. It would be of interest to learn if more sophisticated treatments of the superconducting state, particularly through the inclusion of the anisotropy in the mass renormalization in the normal channel, and more sophisticated treatments of the Coulomb repulsion, would verify this conclusion, and if so, what values for T_c would be predicted.

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APPENDIX A: APPROXIMATE T_c EQUATIONS

For isotropic superconductors, Leavens and Carbotte[18] have produced an approximate T_c equation which is at least as accurate as the famous McMillan equation[20] for most cases considered to date. Carbotte and Daams[19] have generalized it to the case of small anisotropy using the separable model, evaluating the enhancement of T_c to $O(\langle a^2\rangle/[\lambda-\mu^*(\omega_m)])$. In this appendix it is further generalized to all orders of anisotropy, and then through further simplifications it is reduced to simpler equations referred to in the text. Finally the McMillan equation is exhibited, for comparison.

The imaginary axis equivalent of the essential approximation of Leavens and Carbotte is the approximate evaluation

$$\pi T_c=\sum_{q=-N}^{N}\frac{\lambda(p-q)}{|\tilde{\omega}(q)|}\simeq\frac{-\bar{\lambda}+\lambda f}{1+\lambda}\ , \tag{A1}$$

with $f=\ln(1.13\omega_m/T_c)$ as before, with λ the usual electron-phonon parameter, and $\bar{\lambda}$ defined in a similar way,

$$\bar{\lambda}=2\int_0^{\omega_m}d\omega\frac{\alpha^2F(\omega)}{\omega}\ln\left[1+\frac{\omega_m}{\omega}\right]. \tag{A2}$$

[For the $\alpha^2F(\omega)$ used in Sec. II, $\bar{\lambda}=0.386$.] The cutoff frequency in all sums is the maximum phonon frequency $\omega_{co}=\omega_m$. Writing $\tilde{\Delta}_{\vec{k}}(n)=\tilde{\Delta}_0+a_{\vec{k}}\tilde{\Delta}_1$, then Eq. (6) takes the form

$$\tilde{\Delta}_0=\tilde{\Delta}_1-\mu^*(\omega_m)f\left\langle\frac{\tilde{\Delta}_0+a_{\vec{k}}\tilde{\Delta}_1}{1+\lambda(1+a_{\vec{k}})}\right\rangle, \tag{A3}$$

$$\tilde{\Delta}_1=(-\bar{\lambda}+\lambda f)\left\langle\frac{(1+a_{\vec{k}})(\tilde{\Delta}_0+a_{\vec{k}}\tilde{\Delta}_1)}{1+\lambda(1+a_{\vec{k}})}\right\rangle. \tag{A4}$$

Introducing averages similar to those in Eq. (13),

$$r=\left\langle \frac{1}{1+\lambda(1+a_{\vec{k}})} \right\rangle, \quad s=\left\langle \frac{a_{\vec{k}}}{1+\lambda(1+a_{\vec{k}})} \right\rangle, \quad t=\left\langle \frac{a_{\vec{k}}^2}{1+\lambda(1+a_{\vec{k}})} \right\rangle, \tag{A5}$$

allows one to express (A3) and (A4) as

$$[1+\mu^*(\omega_m)rf]\tilde{\Delta}_0-[1-\mu^*(\omega_m)sf]\tilde{\Delta}_1=0, \tag{A6}$$

$$-(r+s)(-\bar{\lambda}+\lambda f)\tilde{\Delta}_0+[1-(s+t)(-\bar{\lambda}+\lambda f)]\tilde{\Delta}_1=0. \tag{A7}$$

Imposing the requirement of a nontrivial solution on (A6) and (A7) produces a quadratic equation for f. Taking the larger root, which is always positive as long as $\lambda>\mu^*(\omega_m)$ or $\langle a^2\rangle>0$, and relating r and s to t, the T_c equation is

$$T_c=1.13\omega_m e^{-f}, \tag{A8}$$

$$f=\frac{-b+\{b^2+4\lambda\mu^*(\omega_m)t[1+\lambda+\bar{\lambda}(1+t/(1+\lambda))]\}^{1/2}}{2\lambda\mu^*(\omega_m)t}, \tag{A9}$$

$$b=\lambda\left[1+\frac{t}{1+\lambda}\right]-\mu^*(\omega_m)\left[1+\lambda^2\frac{t}{1+\lambda}\right]-\bar{\lambda}\mu^*(\omega_m)t. \tag{A10}$$

The parameter t cannot be related exactly to $\langle a^2\rangle$ without assuming details about the anisotropy function $a_{\vec{k}}$. However, this is not significant, because it is given approximately by

$$t\simeq\frac{\langle a^2\rangle}{1+\lambda}+O\left[\frac{\lambda\langle a^3\rangle}{(1+\lambda)^2}\right], \tag{A11}$$

and the correction is always small, independent of $\mu^*(\omega_m)$.

The result of Carbotte and Daams[19] is recovered by expanding the square root in (A9), resulting in

$$f\simeq\frac{1+\lambda+\bar{\lambda}}{\lambda-\mu^*(\omega_m)}-\frac{[\lambda(1+\mu^*(\omega_m))+\bar{\lambda}\mu^*(\omega_m)]^2}{(1+\lambda)[\lambda-\mu^*(\omega_m)]^3}\langle a^2\rangle, \tag{A12}$$

and then evaluating (A8) to first order in $\langle a^2\rangle$ [provided that $\lambda-\mu^*(\omega_m)$ is not too small]. The original Leavens-Carbotte result is trivially obtained from (A12) by setting $\langle a^2\rangle=0$.

Another set of equations which keeps the anisotropy to all orders is obtained as follows. First, $\bar{\lambda}$ is ignored in (A2) and (A3). Second, the renormalization $1+\lambda(1+a_{\vec{k}})$ is dropped in the normal channel, i.e., $r=1$, $s=0$, and $t=\langle a^2\rangle$. The result of Whitmore and Carbotte is recovered, with λ identified as $N(0)V_{e\text{-ph}}$,

$$f=\frac{-b+\{b^2+4\lambda\mu^*(\omega_m)\langle a^2\rangle\}^{1/2}}{2\lambda\mu^*(\omega_m)\langle a^2\rangle}, \tag{A13}$$

with

$$b=(1+\langle a^2\rangle)\lambda-\mu^*. \tag{A14}$$

Finally, the isotropic equation of McMillan is[20,27]

$$T_c=(\langle\omega\rangle/1.20)e^{-f}, \tag{A15}$$

$$f=\frac{1.04(1+\lambda)}{\lambda-\mu^*(\omega_{co})(1+0.62\lambda)}, \tag{A16}$$

with $\langle\omega\rangle$ an average phonon frequency defined using $\alpha^2F(\omega)$. The cutoff frequency is generally taken to be on the order of $10\omega_m$, so that the denominator of Eq. (A15) can be much smaller than that appearing in equations based on the procedure of Leavens and Carbotte.

APPENDIX B: CONDITIONS FOR POSITIVE EIGENVALUES

The basis for part of Sec. III is the conditions under which a matrix has either one, or two or more, nonnegative eigenvalues.

A necessary and sufficient condition for a Hermitian matrix $\underline{A}$ to be nonpositive definite[25,28] (no positive eigenvalues), is that the leading principal minors M_n be either zero or satisfy $\mathrm{sgn}(M_n)=(-1)^{n+1}$. The M_n are the leading subdeterminants, i.e., if the elements of $\underline{A}$ are a_{ij}, then

$$M_0=a_{00}, \quad M_1=\begin{vmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{vmatrix},$$

etc. Note that by a relabeling of the basis functions, any diagonal element can be brought into the a_{00} position. Thus we have the result that if any diagonal element is positive, or if even one of the M_n satisfy $\mathrm{sgn}(M_n)=(-1)^n$, then there is at least one positive eigenvalue.

Now a second theorem can be used to determine if a finite T_c persists for arbitrarily large $\mu^*(\omega_m)$, given a specified anisotropy in the attractive part of the electron-electron interaction. The basis is the Courant-Fisher theorem,[28] which states the following.

If $\underline{A}$ is a real symmetric matrix with eigenvalues $e_1\geq e_2\geq\cdots\geq e_n$, $\underline{B}$ is a non-negative definite matrix of rank r, with $1\leq r\leq n$, and the ordered eigenvalues of $\underline{A}+\underline{B}$ are labeled $f_1\geq f_2\geq\cdots\geq f_n$, then

(1) $f_i\geq e_i$, $i=1,\ldots,n$

(2) $f_i\leq e_{i-r}$, $i=r+1,\ldots,n$.

This can be easily generalized to the case where $\underline{B}$ is nonpositive definite of rank satisfying $1\leq r\leq n$, in which case

(1) $f_i \leq e_i$, $i=1,\ldots,n$

(2) $f_i \leq e_{i+r}$, $i=1,\ldots,n-r$.

In the context of Sec. II, μ^* is assumed constant, so that $\mu^*_{ll'}$ is a matrix of rank 1 (even when there is more than one piece to the Fermi surface). This means the largest eigenvalue of $\kappa_{ll'}$ must be at least as large as the second largest eigenvalues of $\lambda_{ll'}$, so superconductivity would persist for arbitrary μ^*.

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