Anisotropic superconductors with repulsive average interaction

M. D. Whitmore
Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada A1B 3X7

J. P. Carbotte
Department of Physics, McMaster University, Hamilton, Ontario, Canada L8S 4M1

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Using Bardeen-Cooper-Schrieffer theory with a model interaction given by an anisotropic, separable attraction plus an isotropic repulsion, we obtain an expression for the superconducting transition temperature T_c. It is found that, as long as some anisotropy is present, $T_c > 0$ for all values of μ^*, even when on average the effective electron-electron interaction is repulsive. Further, in this regime, T_c depends strongly on the mean-square anisotropy, $\langle a^2 \rangle$. The free energy is also considered briefly and shown to be less than that of the normal state. This represents a new criterion for the stability of the superconducting state relative to the normal state.

I. INTRODUCTION

Recent solutions of the anisotropic Eliashberg gap equations for materials with paramagnetic impurities have indicated an enhancement of the anisotropy[1,2] and a corresponding effect on the superconducting transition temperature T_c. This leads to the speculation that certain pure materials which would not otherwise superconduct at a measurable temperature, may in fact do so because of the anisotropy. The further possibility exists that even if on average the Coulomb repulsion between electrons is stronger than the effective attraction induced by the electron-phonon interaction, a finite and measurable T_c may still occur.

To investigate this, we consider BCS theory in which the effective electron-electron interaction is represented by a separable attractive part, and the repulsion by an isotropic term.

$$V_{\vec{k}\vec{k}'} = (1 + a_{\vec{k}}) V_{ep} (1 + a_{\vec{k}'}) - V_C \quad . \tag{1}$$

Both V_{ep} and V_C are assumed greater than zero. The anisotropy is represented by the $a_{\vec{k}}$, which when averaged over the Fermi surface gives zero, i.e.,

$$\int \frac{d\Omega_{\vec{k}}}{4\pi} a_{\vec{k}} = 0 \quad . \tag{2}$$

Physically, one expects the first term in Eq. (1) to be due to the electron-phonon interaction, and the second due to the Coulomb repulsion. However, one could envisage each term as containing some of each of these effects; for example, anisotropy in V_C could be incorporated in the first term, and differences between the anisotropic and the isotropic parts of the electron-phonon interaction which are not adequately represented through the separable model might be included through a modification to V_C.

The double Fermi-surface average of $V_{\vec{k}\vec{k}'}$ is given by

$$\langle V_{\vec{k}\vec{k}'} \rangle = \int \frac{d\Omega_{\vec{k}}}{4\pi} \frac{d\Omega_{\vec{k}'}}{4\pi} (1 + a_{\vec{k}}) V_{ep} (1 + a_{\vec{k}'}) - V_C$$

$$= V_{ep} - V_C \quad . \tag{3}$$

In the absence of anisotropy ($a_{\vec{k}} = 0$), BCS theory predicts

$$k_B T_c = 1.13 \hbar \omega_D \exp\left[- \frac{1}{N(0)(V_{ep} - V_C)} \right] \quad , \tag{4}$$

so that $T_c \to 0$ as $V_C \to V_{ep}$. Markowitz and Kadanoff[3] have considered another simpler version of Eq. (1) in which $V_C = 0$, and found

$$k_B T_c = 1.13 \hbar \omega_D \exp\left[- \frac{1}{N(0) V_{ep} (1 + \langle a^2 \rangle)} \right] \quad , \tag{5}$$

where

$$\langle a^2 \rangle = \int \frac{d\Omega_{\vec{k}}}{4\pi} a_{\vec{k}}^2 \quad . \tag{6}$$

Within each of these models, the average interaction must be attractive for a nonzero T_c. In the next section we work out T_c when both $a_{\vec{k}}$ and V_C are nonzero, and show that for any V_C, $T_c > 0$ as long as $\langle a^2 \rangle \neq 0$; of course for large V_C, T_c is found to be very small. Although this is perhaps a surprising result, it is not without precedent. Kohn and Luttinger[4] argued that even when the electrons in a metal interact only through a screened Coulomb interaction, by taking advantage of the attractive region caused by the Friedel oscillations, Cooper pairs can be formed; thus giving rise to superconductivity. The anticipated T_c's, though low, were finite.

II. BCS THEORY OF T_c

We first derive the general expression for T_c, and then consider certain limiting forms. As will be seen a little later, focusing attention on the regime $V_C \gtrsim V_{ep}$ implies restricting interest primarily to the weak-coupling limit, where the use of the BCS theory is valid.

With $V_{kk'}$ given by Eq. (1) the usual BCS gap equation is

$$\Delta_{\vec{k}} = \sum_{\vec{k}'}' [V_{ep}(1+a_{\vec{k}'}) - V_C]\left[\Delta_{\vec{k}'}\frac{1-2f(E_{\vec{k}'})}{2E_{\vec{k}'}}\right] + a_{\vec{k}}\sum_{\vec{k}'}' V_{ep}(1+a_{\vec{k}'})\Delta_{\vec{k}'}\frac{1-2f(E_{\vec{k}'})}{2E_{\vec{k}'}} \ , \tag{7}$$

where $E_{\vec{k}'} = (\epsilon_{\vec{k}'}^2 + \Delta_{\vec{k}'}^2)^{1/2}$ and the prime on the sum indicates it is restricted to the region $|\epsilon_{\vec{k}}| \leq \hbar\omega_D$, $|\epsilon_{\vec{k}'}| \leq \hbar\omega_D$, where $\hbar\omega_D$ is the Debye frequency. Clearly $\Delta_{\vec{k}}$ has the form

$$\Delta_{\vec{k}} = \Delta_{\vec{k}}^0 + a_{\vec{k}}\Delta_{\vec{k}}' \ . \tag{8}$$

We now specialize to T_c, in which case Eq. (7) can be linearized in the usual fashion by setting $\Delta_{\vec{k}}^2 = 0$. Substituting Eq. (8) into the linearized equation we then obtain

$$\Delta_{\vec{k}}^0 + a_{\vec{k}}\Delta_{\vec{k}}' = \sum_{\vec{k}'}' [V_{ep}(1+a_{\vec{k}'}) - V_C](\Delta_{\vec{k}'}^0 + a_{\vec{k}'}\Delta_{\vec{k}'}')\frac{\tanh(\frac{1}{2}\beta_c|\epsilon_{\vec{k}'}|)}{2|\epsilon_{\vec{k}'}|}$$
$$+ a_{\vec{k}}\sum_{\vec{k}'}' V_{ep}(1+a_{\vec{k}'})(\Delta_{\vec{k}'}^0 + a_{\vec{k}'}\Delta_{\vec{k}'}')\frac{\tanh(\frac{1}{2}\beta_c|\epsilon_{\vec{k}'}|)}{2|\epsilon_{\vec{k}'}|} \ , \tag{9}$$

where $\beta_c = 1/k_B T_c$. The next step is changing the sum over $\vec{k}$ to multiple integrals, resulting in

$$\Delta_{\vec{k}}^0 + a_{\vec{k}}\Delta_{\vec{k}}' = \int_{-\hbar\omega_D}^{\hbar\omega_D} N(\epsilon_{\vec{k}'})\, d\epsilon_{\vec{k}'}\frac{\tanh(\frac{1}{2}\beta_c|\epsilon_{\vec{k}'}|)}{2|\epsilon_{\vec{k}'}|}\int\frac{d\Omega_{\vec{k}'}}{4\pi}[V_{ep}(1+a_{\vec{k}'}) - V_C](\Delta_{\vec{k}'}^0 + a_{\vec{k}'}\Delta_{\vec{k}'}')$$
$$+ a_{\vec{k}}\int_{-\hbar\omega_D}^{\hbar\omega_D} N(\epsilon_{\vec{k}'})\, d\epsilon_{\vec{k}'}\frac{\tanh(\frac{1}{2}\beta_c|\epsilon_{\vec{k}'}|)}{2|\epsilon_{\vec{k}'}|}\int\frac{d\Omega_{\vec{k}'}}{4\pi}V_{ep}(1+a_{\vec{k}'})(\Delta_{\vec{k}'}^0 + a_{\vec{k}'}\Delta_{\vec{k}'}') \ . \tag{10}$$

Because the energy integration is over a very small interval on the scale of electron energies, we assume the $a_{\vec{k}}$ has only angular dependence in this region, which implies the same for $\Delta_{\vec{k}}$. Hence $\Delta_{\vec{k}}^0$ and $\Delta_{\vec{k}}'$ are each constant (or zero), and can be written simply as Δ_l.

A further simplification can be made by invoking the usual assumption that $N(\epsilon_{\vec{k}'})$ does not vary in the energy range $\pm\hbar\omega_D$, so can be taken outside the integral. If we then identify $N(0)V_C = \mu^*$, define

$$F = \int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{\tanh(\frac{1}{2}\beta_c|\epsilon|)}{2|\epsilon|}\,d\epsilon \tag{11}$$

and make use of Eq. (11), Eq. (10) simplifies to

$$\Delta_0 + a_{\vec{k}}\Delta_1 = F\{[N(0)V_{ep} - \mu^*]\Delta_0 - N(0)V_{ep}\langle a^2\rangle\Delta_1\}$$
$$+ a_{\vec{k}}FN(0)V_{ep}(\Delta_0 + \langle a^2\rangle\Delta_1) \ , \tag{12}$$

with $\langle a^2\rangle$ given by Eq. (6). Averaging Eq. (12) over the Fermi surface and simplifying, we obtain

$$\{1 - F[N(0)V_{ep} - \mu^*]\}\Delta_0 - [FN(0)V_{ep}\langle a^2\rangle]\Delta_1 = 0 \ . \tag{13}$$

Multiplying Eq. (12) by $a_{\vec{k}}$, averaging and simplifying leads to

$$[-FN(0)V_{ep}]\Delta_0 + [1 - FN(0)V_{ep}\langle a^2\rangle]\Delta_1 = 0 \ . \tag{14}$$

Equations (13) and (14) constitute a pair of homogeneous equations for Δ_0 and Δ_1. They have a nontrivial solution only if the determinant of their coefficients is zero. Imposing this condition, and solving for F we find two possibilities.

$$F=\frac{N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*\pm\{[N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*]^2+4N(0)V_{ep}\mu^*\langle a^2\rangle\}^{1/2}}{-2N(0)V_{ep}\mu^*\langle a^2\rangle} \quad . \tag{15}$$

By inspecting Eq. (11), it can be seen that for T_c real, $F\geq 0$, so we must take only the solution with the negative sign in Eq. (15).

The final expression for T_c can now be obtained. The integral (11) is just the usual one appearing in the BCS theory, with result

$$F\simeq \ln(1.13\hbar\omega_D/k_BT_c) \quad , \tag{16}$$

so that

$$k_BT_c=1.13\hbar\omega_De^{-F} \quad . \tag{17}$$

In certain limiting cases, Eq. (17) must reduce to known expressions. It is straightforward to show that when

$$\frac{N(0)V_{ep}\mu^*\langle a^2\rangle}{[N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*]^2}\ll 1 \tag{18}$$

then

$$F\simeq\begin{cases} +\dfrac{1}{N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*}, & N(0)V_{ep}(1+\langle a^2\rangle)>\mu^* \\ -\dfrac{N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*}{N(0)V_{ep}\mu^*\langle a^2\rangle}, & N(0)V_{ep}(1+\langle a^2\rangle)<\mu^* \quad . \end{cases} \tag{19}$$

From this it is clear that in the isotropic case, the usual BCS expression [Eq. (4)] is recovered, and that in the anisotropic case in which $\mu^*=0$, the result of Markowitz and Kadanoff [Eq. (5)] is obtained.

In closing this section we return to the question of the applicability of BCS theory. Having identified μ^*, Eq. (3) can now be written

$$N(0)\langle V_{\vec{k}\vec{k}'}\rangle=N(0)V_{ep}-\mu^* \quad . \tag{20}$$

Hence focusing of attention to $V_{ep}\simeq V_C$ translates to $N(0)V_{ep}\simeq\mu^*$, and since μ^* is generally $\lesssim 0.2$, this is the weak-coupling range.

III. FREE ENERGY AND CRITICAL MAGNETIC FIELD

Before proceeding to presentation and discussion of the results for T_c in this model, we consider the free energy. An analytic expression for zero temperature is first obtained, and then it is shown that for any $T<T_c$, the free energy of the superconducting state is less than that of the normal state.

The following expression for the electron free energy,[5]

$$\Omega=-2k_BT\sum_{\vec{k}}\ln(1+e^{-\beta E_{\vec{k}}}) + \sum_{\vec{k}}\left(\epsilon_{\vec{k}}-E_{\vec{k}}+\Delta_{\vec{k}}^2\frac{1-2f(E_{\vec{k}})}{2E_{\vec{k}}}\right) \quad , \tag{21}$$

is valid for both the superconducting state, and the normal state for which one uses $\Delta_{\vec{k}}=0$. At zero temperature, the difference in free energy $\Delta\Omega=\Omega_s-\Omega_N$ is

$$\Delta\Omega=\sum_{\vec{k}}'\left(|\epsilon_{\vec{k}}|-E_{\vec{k}}+\frac{\Delta_{\vec{k}}^2}{2E_{\vec{k}}}\right) \quad , \tag{22}$$

which can be conveniently expressed as

$$\Delta\Omega=2N(0)\int\frac{d\Omega_{\vec{k}}}{4\pi}\int_0^{\hbar\omega_D}d\epsilon_{\vec{k}}\left(\epsilon_{\vec{k}}-(\epsilon_{\vec{k}}^2+\Delta_{\vec{k}}^2)^{1/2}+\frac{\Delta_{\vec{k}}^2}{2(\epsilon_{\vec{k}}^2+\Delta_{\vec{k}}^2)^{1/2}}\right) \quad . \tag{23}$$

Performing the energy integral first, and using the fact that $\hbar\omega_D\gg\Delta_{\vec{k}}$, this becomes

$$\Delta\Omega=-N(0)\int\frac{d\Omega_{\vec{k}}}{4\pi}\frac{\Delta_{\vec{k}}^2}{2} \tag{24}$$

$$=\frac{N(0)}{2}(\Delta_0^2+\langle a^2\rangle\Delta_1^2) \quad . \tag{25}$$

The zero-temperature critical magnetic field $H_c(0)$ is then given by

$$\frac{H_c(0)^2}{8\pi} = \frac{N(0)}{2}(\Delta_0^2 + \langle a^2\rangle \Delta_1^2) \ . \tag{26}$$

At finite T an analytic form for Ω_s cannot be derived. However, consider the difference $\Delta\Omega$, which can be expressed using Eq. (21) as

$$\Delta\Omega = \sum_{\vec{k}}{}' \left[-2k_B T \ln\left(\frac{1+e^{-\beta E_{\vec{k}}}}{1+e^{-\beta|\epsilon_{\vec{k}}|}} \right) + |\epsilon_{\vec{k}}| - E_{\vec{k}} + \Delta^2_{\vec{k}} \frac{\tanh(\frac{1}{2}\beta E_{\vec{k}})}{2E_{\vec{k}}} \right] . \tag{27}$$

A sufficient condition ensuring this difference to be negative is that each term in the sum be no greater than zero:

$$-2k_B T \ln\left(\frac{1+e^{\beta E_{\vec{k}}}}{1+e^{-\beta|\epsilon_{\vec{k}}|}} \right) + |\epsilon_{\vec{k}}| - E_{\vec{k}} + \Delta^2_{\vec{k}} \frac{\tanh(\frac{1}{2}\beta E_{\vec{k}})}{2E_{\vec{k}}} \leq 0 \ . \tag{28}$$

This can be simplified to the condition

$$\cosh\left(\frac{\beta E_{\vec{k}}}{2}\right) \geq \cosh\left(\frac{\beta|\epsilon_{\vec{k}}|}{2}\right)\left(\frac{\beta\Delta^2_{\vec{k}}}{4E_{\vec{k}}} \tanh\frac{\beta E_{\vec{k}}}{2}\right) \tag{29}$$

which can be verified numerically in a straightforward manner. Hence this state is of lower free energy than the normal state.

IV. RESULTS AND DISCUSSION

The main numerical results are summarized in Figs. 1 and 2. In the first of these, $N(0)V_{ep} = 0.28$ and $\hbar\omega_D = 32$ meV which gives a T_c corresponding approximately to Al for $\mu^* = 0.13$ and in the second $N(0)V_{ep} = 0.40$ and $\hbar\omega_D = 21$ meV which gives approximately the T_c of Nb for $\mu^* = 0.12$.

In each case the variation of T_c with μ^* is shown for different values of $\langle a^2\rangle$. The point $\mu^*/N(0)V_{ep} = 1$ corresponds to a potential which on average is neutral. For large $\langle a^2\rangle$, T_c can remain 0.1 K for the first example, and 0.7 K for the second. In fact, T_c remains above 1 mK well into the region $\mu^* > N(0)V_{ep}$, where the potential is on average repulsive. We note further that for no value of μ^* does T_c become zero, so long as $\langle a^2\rangle$ is greater than zero.

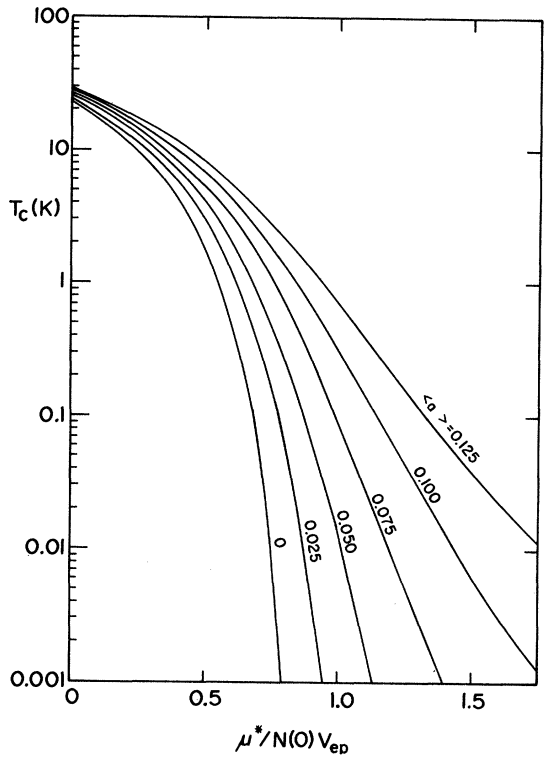

FIG. 1. T_c as a function of μ^* for different values of $\langle a^2\rangle$. The different curves correspond to values of $\langle a^2\rangle$ of 0, 0.025, 0.050, 0.075, 0.100, and 0.125. The region to the right of $\mu^* N(0)V_{ep} = 1$ represents a potential which is on average repulsive. The parameters $N(0)V_{ep}$ and $\hbar\omega_D$ correspond approximately to aluminum.

It is clear from these figures that T_c depends sensitively on $\langle a^2\rangle$ in these regions. For example, at $\mu^* = N(0)V_{ep}$ changing $\langle a^2\rangle$ from 0.075 to 0.100 increases T_c by a factor of about 6 for the first material, and for $\mu^* > N(0)V_{ep}$ the effect is even greater. This can be understood by examining the expression for T_c for the case $\mu^* = N(0)V_{ep}$. To leading order in the anisotropy, it becomes

$$k_B T_c = 1.13\hbar\omega_D \exp\left(\frac{1}{N(0)V_{ep}\langle a^2\rangle^{1/2}}\right) \ . \tag{30}$$

This equation exhibits two interesting features. First it is clear that because the anisotropy enters in the same way as V_{ep}, it cannot be treated as a small perturbation in V_{ep}. Second, the fact that it is $\langle a^2\rangle^{1/2}$ and not $\langle a^2\rangle$ which is important here, is clearly responsible for T_c being as large as it is. Another measure of this sensitivity is the partial derivative of T_c with respect to μ^*, evaluated at $\mu^* = N(0)V_{ep}$, which is given by

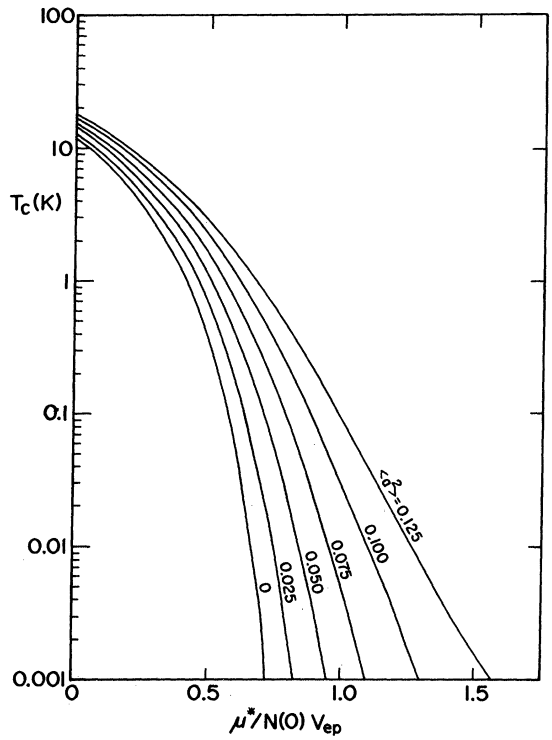

FIG. 2. T_c as a function of μ^* for different values of $\langle a^2\rangle$. The curves are the same as in Fig. 1, except that $N(0)V_{ep}$ and $\hbar\omega_D$ correspond approximately to niobium.

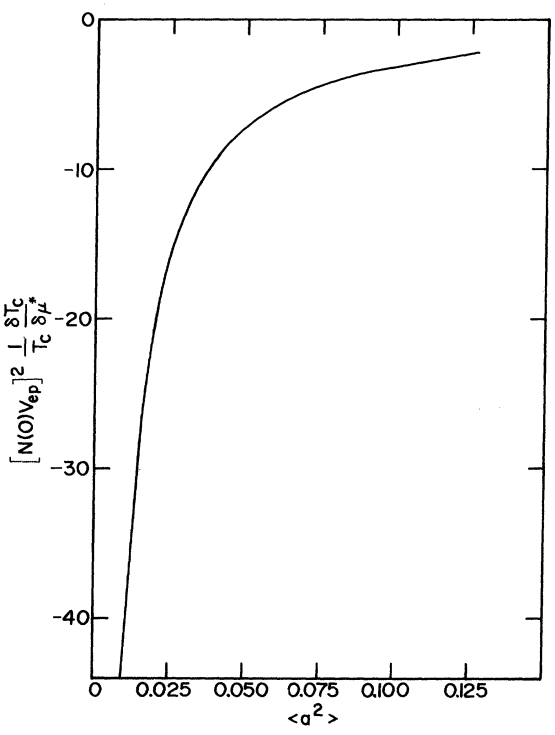

FIG. 3. Partial derivative of T_c with respect to μ^*, given by Eq. (31) of the text. The limiting behavior, Eq. (32), is also apparent.

$$\left[\frac{1}{T_c}\left(\frac{\partial T_c}{\partial \mu^*}\right)\right]_{\langle a^2\rangle|\mu^*=N(0)V_{ep}} = -\frac{1}{2[N(0)V_{ep}]^2\langle a^2\rangle}(1+\langle a^2\rangle) - \frac{\langle a^2\rangle(\langle a^2\rangle+3)}{[\langle a^2\rangle(\langle a^2\rangle+4)]^{1/2}} \quad . \tag{31}$$

This function has the interesting limiting behavior

$$\left[\frac{1}{T_c}\left(\frac{\partial T_c}{\partial \mu^*}\right)\right]_{\langle a^2\rangle|\mu^*=N(0)V_{ep}} \rightarrow \begin{cases} -\dfrac{1}{2(N(0)V_{ep})^2\langle a^2\rangle}, & \text{as } \langle a^2\rangle \rightarrow 0 \\ 0, \text{ as } \langle a^2\rangle \rightarrow \infty \ , \end{cases} \tag{32}$$

which agrees with the very rapid decrease of T_c with μ^* for small $\langle a^2\rangle$, but slower one for larger $\langle a^2\rangle$. The full function (31) is illustrated in Fig. 3.

The strong dependence of T_c on $\langle a^2\rangle$ suggests this state will be very sensitive to the presence of nonmagnetic impurities, which are known to wash out the anisotropy. This matter has been investigated, and will be the subject of an ensuing publication.[6] Briefly the result is that for T_c to remain above 1 mK, with $\mu^* > N(0)V_{ep}$, the concentration of impurities must be no more than about 0.001% to 0.01%, depending on the material.

Systems with electron-phonon mass enhancement factor λ comparable to μ^* are found in the alkalis with $\lambda \sim 0.11$ to 0.19,[7] and the noble metals ($\lambda N 0.16$ to 0.21).[8] Further, Daams, Mitrović, and Carbotte[9] have shown that the effects of paramagnons in metals can be simulated by an effective $\lambda_{\text{eff}} = \lambda/(1+\lambda_s)$ and $\mu^*_{\text{eff}} = (\mu^* + \lambda_s)/(1+\lambda_s)$ where λ_s is the paramagnon mass renormalization. Since λ_s can be at least as large as 0.3,[10] $\lambda_{\text{eff}} \sim \mu^*_{\text{eff}}$ could be realized.

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