

Some properties of superconducting virtual-bound-state alloys

Yutaka Okabe* and A. D. S. Nagi

Guelph-Waterloo Program for Graduate Work in Physics, Department of Physics, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

(Received 21 March 1983)

Using the Anderson model in the nonmagnetic limit, we have calculated some properties of the superconducting virtual-bound-state alloys. The calculated properties are the transition temperature T_c , the jump in specific heat at T_c , ΔC , the electronic density of states, and the tunneling conductance. Special attention is paid to the systematic variation of these properties with the resonance width Γ . It is found that the initial slope of the normalized ΔC versus the normalized T_c curve has a maximum value of 3.638, which is the highest value reported in the literature for the impurity problem. Our tunneling study suggests that for an electron-tunneling search of bound states in alloys with relatively large Γ , an ultra-low-temperature experiment is desirable.

I. INTRODUCTION

Recent work of Terris and Ginsberg¹ and that of Salomaa and Nieminen² have renewed interest in the study of the superconducting virtual-bound-state alloys. In Ref. 1 an electron-tunneling search of the bound states in superconducting Al-Mn was carried out with negative results. In Ref. 2, the Anderson model³ was used to describe the impurities. In this model,⁴ a d -electron state localized on a transition-metal impurity atom hybridizes with the conduction-electron states of the host material leading to a localized resonance of width Γ . There is a Coulomb repulsion U between localized resonances of opposite spin. Whether the impurity behaves nonmagnetically or magnetically depends on the value of $U/\pi\Gamma$. With $U=0$, one has the nonmagnetic limit of the Anderson impurity. By using this limit, it was shown in Ref. 2 that for a finite impurity concentration, there is an impurity band within the BCS energy gap. The possibility of such a band was first suggested by Machida and Shibata.⁵

On the theoretical side, a pioneering study on this topic was done by Zuckerman.⁶ Other notable related works are by Ratto and Blandin,⁷ Kiwi and Zuckermann,⁸ Kaiser,⁹ and Shiba.¹⁰ The difference between the earlier studies and that of Ref. 2 for $U=0$ is that, whereas in most of the earlier works the resonance width Γ was taken much larger than the Debye cutoff frequency ω_D , in the recent investigation the region $\Gamma \sim T_c$ was explored in order to clarify the existence of bound states.

Because of the recent interest in this problem, the present study has been carried out. We have calculated the transition temperature T_c , the jump in specific heat at T_c , ΔC , the initial slope of the specific-heat jump versus T_c curve, the electronic density of states, and the tunneling conductance by paying attention to their systematic variation with respect to Γ . We find interesting behavior in T_c and ΔC , especially for small Γ . For example, the maximum value of the initial slope of ΔC -vs- T_c curve is the highest for the impurity problem. We also make a

comment on the experimental research. A preliminary study of the specific-heat jump has been reported earlier.¹¹

II. TRANSITION TEMPERATURE AND SPECIFIC-HEAT JUMP

Let us consider a random distribution of d -state impurities in a BCS superconductor. Describing the impurities by using the Anderson model with $U=0$ and neglecting the impurity-impurity interaction, the single-particle Green's function for the conduction electrons of the host metal is

$$G(\vec{k}, \omega_n) = (\tilde{\omega}_n - \epsilon_{\vec{k}} \tau_3 + \tilde{\Delta}_n \tau_1)^{-1}, \quad (1)$$

where $\omega_n = \pi T(2n+1)$ (with T as temperature and n as an integer), $\epsilon_{\vec{k}}$ is the Bloch-state energy, τ_i are Pauli spin matrices, and the parameter $U_n = \tilde{\omega}_n / \tilde{\Delta}_n$ satisfies equation

$$U_n = \frac{\omega_n}{\Delta} + \frac{n_i \Gamma}{\pi N_0 \Delta} \frac{\omega_n}{\Gamma^2 + E_d^2 + \omega_n^2 + 2\Gamma \omega_n U_n (1 + U_n^2)^{-1/2}}. \quad (2)$$

In Eq. (2), Δ is the impurity- and temperature-dependent superconducting order parameter, n_i is the impurity concentration, N_0 is the single-spin density of electron states at the Fermi level in the normal metal, $\Gamma = \pi N_0 \langle V_{kd}^2 \rangle$ is the half-width of the d resonance with V_{kd} as the admixture matrix element between d state and the conduction electrons, and E_d is the displacement of the center of the resonance from the Fermi level.

First we discuss the thermodynamic properties. The order parameter satisfies the self-consistency equation

$$\Delta = 2\pi T g N_0 \sum_{n=0}^{\bar{n}} (1 + U_n^2)^{-1/2}, \quad (3)$$

where g is the BCS interaction constant and $\bar{n} = \omega_D / 2\pi T$ with ω_D as the Debye cutoff frequency.

Now one has the BCS relation

$$1/gN_0 = \ln(2\gamma_e \omega_D / \pi T_{c0}),$$

where T_{c0} is T_c (the transition temperature) in the absence of impurities and $\ln \gamma_e$ is Euler's constant. Also,

$$\ln(2\gamma_e \omega_D / \pi T) = 2\pi T \sum_{n=0}^{\bar{n}} (1/\omega_n).$$

Using these two relations in Eq. (3), we obtain

$$\ln(T/T_{c0}) = 2\pi T \sum_{n=0}^{\infty} [(1/\Delta)(1+U_n^2)^{-1/2} - (1/\omega_n)]. \tag{4}$$

For T near T_c , Δ becomes small and $U_n \gg 1$. Then Eq. (2) gives

$$U_n = a_{-1} \frac{1}{\Delta} + a_1 \Delta + \dots, \tag{5}$$

with

$$a_{-1} = \omega_n \left[1 + \frac{\gamma}{E_d^2 + (\Gamma + \omega_n)^2} \right], \tag{6}$$

$$a_1 = \frac{\gamma \Gamma}{[E_d^2 + (\Gamma + \omega_n)^2 + \gamma]^2},$$

where

$$\gamma = n_i \Gamma / \pi N_0. \tag{7}$$

Using Eqs. (4) and (5), we obtain

$$\ln(T_{c0}/T) = B_0(n_i, T) + \frac{1}{2} B_1(n_i, T) (\Delta/2\pi T)^2 + \dots, \tag{8}$$

where

$$B_0(n_i, T) = 2\pi T \sum_{n=0}^{\infty} \left[\frac{1}{\omega_n} - \frac{1}{a_{-1}} \right], \tag{9}$$

$$B_1(n_i, T) = (2\pi T)^3 \sum_{n=0}^{\infty} \left[2a_1 + \frac{1}{a_{-1}} \right] \left[\frac{1}{a_{-1}} \right]^2.$$

As shown in the Appendix, the quantities $B_0(n_i, T)$ and $B_1(n_i, T)$ can be written as

$$B_0(n_i, T) = \frac{\gamma}{\Gamma^2 + \alpha^2} \left[\operatorname{Re} \psi \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] - \psi \left(\frac{1}{2} \right) - \frac{\Gamma}{\alpha} \operatorname{Im} \psi \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] \right], \tag{10}$$

$$B_1(n_i, T) = -\frac{D_1}{2} \psi^{(2)} \left(\frac{1}{2} \right) + D_2 (2\pi T) \psi^{(1)} \left(\frac{1}{2} \right) + \operatorname{Re} \left\{ \frac{D_3}{12\pi T} \psi^{(3)} \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] - \frac{D_4}{2} \psi^{(2)} \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] + D_5 (2\pi T) \psi^{(1)} \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] - D_6 (2\pi T)^2 \left[\psi \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] - \psi \left(\frac{1}{2} \right) \right] \right\}, \tag{11}$$

where D_i ($i=1, 2, \dots, 6$) are defined in Eqs. (A6), $\alpha = (E_d^2 + \gamma)^{1/2}$, $\psi^{(n)}(z)$ are polygamma functions,¹² and Re (Im) stands for the real (imaginary) part of the functions.

The equation for T_c is obtained by setting $\Delta=0$ in Eq. (8) and is

$$\ln(T_{c0}/T_c) = B_0(n_i, T_c). \tag{12}$$

The dependence of T_c on the impurity concentration is computed using Eqs. (12) and (10). For the symmetric case ($E_d=0$) such a dependence is shown in Fig. 1 for $\Gamma/\Delta_0(0)=1.0, 5.0,$ and 25.0 . Here $\Delta_0(0)$ is the zero-temperature order parameter in the absence of impurities.

Let us consider the low impurity concentration behavior in detail. For a low impurity concentration, Eqs. (12) and (10) can be written as

$$T_c/T_{c0} = 1 - n_i b_0 + O(n_i^2), \tag{13}$$

where b_0 represents the initial slope of the T_c/T_{c0} -vs- n_i curve. Further,

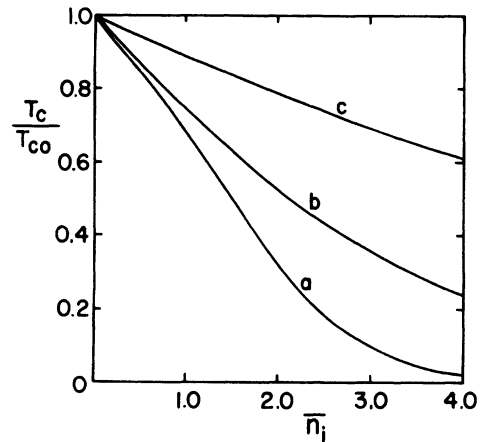


FIG. 1. Normalized transition temperature T_c/T_{c0} vs the normalized impurity concentration \bar{n}_i [$=n_i/\pi N_0 \Delta_0(0)$] for $\Gamma=1.0$ (curve a), 5.0 (curve b), and 25.0 (curve c). Here $\Gamma = \Gamma/\Delta_0(0)$ with Γ as the half-width of the resonance level and $\Delta_0(0)$ as the zero-temperature BCS order parameter. In all figures we have taken $E_d=0$ (symmetric case).

$$b_0 = \lim_{n_i \rightarrow 0} \left[\frac{\partial}{\partial n_i} B_0(n_i, T) \right]$$

$$= \frac{\Gamma}{\pi N_0 (\Gamma^2 + E_d^2)} \left[\operatorname{Re} \psi \left[\frac{1}{2} + \frac{\Gamma + iE_d}{2\pi T_{c0}} \right] - \psi \left(\frac{1}{2} \right) - \frac{\Gamma}{E_d} \operatorname{Im} \psi \left[\frac{1}{2} + \frac{\Gamma + iE_d}{2\pi T_{c0}} \right] \right]. \quad (14)$$

For $|(\Gamma + iE_d)/2\pi T_{c0}| \gg 1$, Eq. (14) gives

$$b_0 = \frac{\Gamma}{\pi N_0 (\Gamma^2 + E_d^2)} \left[\ln \left[\frac{4\gamma_e (\Gamma^2 + E_d^2)^{1/2}}{2\pi T_{c0}} \right] - \frac{\Gamma}{E_d} \arctan \frac{E_d}{\Gamma} \right]. \quad (15)$$

For $|(\Gamma + iE_d)/2\pi T_{c0}| \ll 1$, Eq. (14) gives

$$b_0 = \frac{8\Gamma}{\pi N_0 (2\pi T_{c0})^2} \left[\lambda(3) - 4\lambda(4) \frac{\Gamma}{2\pi T_{c0}} \right], \quad (16)$$

where

$$\lambda(l) = \sum_{n=0}^{\infty} (2n+1)^{-l} = \frac{1}{2^l (-1)^l (l-1)!} \psi^{(l-1)} \left(\frac{1}{2} \right). \quad (17)$$

For given values of $\Gamma/2\pi T_{c0}$ and $E_d/2\pi T_{c0}$, Eqs. (15) and (16) can be used to evaluate the initial slope b_0 . One should note that b_0 becomes smaller for sufficiently small Γ . In Fig. 1 we have only shown the curves for $\Gamma/\Delta_0(0)$ not less than 1.0.

For a large impurity concentration, Eqs. (12) and (10) give

$$\frac{T_c}{T_{c0}} \sim \exp \left[- \frac{\gamma}{E_d^2 + \Gamma^2} \ln \frac{4\gamma_e \gamma^{1/2}}{2\pi T_{c0}} \right]. \quad (18)$$

There is no critical concentration. Such an exponential decrease of T_c was already pointed out in Ref. 9.

The difference in the Helmholtz free-energy density of the alloy in the normal and the superconducting phases for T near T_c is calculated from the relation

$$F_{S-N} = - \frac{N_0}{4} B_1(n_i, T) \frac{\Delta^4}{(2\pi T_c)^2}$$

$$= -N_0 \frac{4\pi^2 T_c^2}{B_1(n_i, T_c)} \left[1 + T_c \frac{\partial}{\partial T} B_0(n_i, T) \right]_{T=T_c}^2$$

$$\times \left[1 - \frac{T}{T_c} \right]^2, \quad (19)$$

where we have used the value of Δ^2 near T_c obtained from Eq. (8).

The specific-heat jump at T_c is obtained from the relation

$$\Delta C = -T_c \left[\frac{\partial^2 F_{S-N}}{\partial T^2} \right]_{T=T_c} \quad (20)$$

and is given by

$$\frac{\Delta C}{\Delta C_0} = \frac{T_c}{T_{c0}} \frac{B_1(0, T_{c0})}{B_1(n_i, T_c)} \left[1 + T_c \frac{\partial B_0(n_i, T_c)}{\partial T_c} \right]^2, \quad (21)$$

where ΔC_0 is the value of ΔC for the pure superconductor, i.e.,

$$\Delta C_0 = 8\pi^2 N_0 T_{c0} / [-\psi^{(2)}(\frac{1}{2}) / 2].$$

In the literature, the specific-heat jump has not been studied except for the limiting cases.^{8,10} Equation (21) with (10) and (11) is a general expression for ΔC .

For a low impurity concentration we can write

$$\left[1 + T_c \frac{\partial B_0(n_i, T_c)}{\partial T_c} \right]^2 = 1 + n_i b_{01} + O(n_i^2), \quad (22)$$

$$\frac{B_1(0, T_{c0})}{B_1(n_i, T_c)} = 1 + n_i b_1 + O(n_i^2), \quad (23)$$

where

$$b_{01} = 2T_{c0} \lim_{n_i \rightarrow 0} \left[\frac{\partial}{\partial n_i} \left[\frac{\partial B_0(n_i, T_c)}{\partial T_c} \right] \right] = \frac{\Gamma}{\pi N_0 (\pi T_{c0} E_d)} \operatorname{Im} \left[\psi^{(1)} \left[\frac{1}{2} + \frac{\Gamma + iE_d}{2\pi T_{c0}} \right] \right], \quad (24)$$

$$b_1 = - \lim_{n_i \rightarrow 0} \left[\frac{\partial}{\partial n_i} \left[\frac{B_1(n_i, T_c)}{B_1(0, T_{c0})} \right] \right]$$

$$= \frac{\Gamma}{\pi N_0} \left[\frac{3}{\Gamma^2 + E_d^2} + \frac{2}{\psi^{(2)}(\frac{1}{2})} \left\{ \frac{16\pi T_{c0} \Gamma}{(\Gamma^2 + E_d^2)^2} \psi^{(1)} \left(\frac{1}{2} \right) - \frac{2\pi T_{c0} \Gamma}{E_d^2} \operatorname{Re} \left[\frac{1}{(\Gamma + iE_d)^2} \psi^{(1)} \left[\frac{1}{2} + \frac{\Gamma + iE_d}{2\pi T_{c0}} \right] \right] \right\} \right.$$

$$\left. - \frac{4\pi^2 T_{c0}^2}{E_d} \operatorname{Re} \left[\left[\frac{3i}{(\Gamma + iE_d)^3} - \frac{2\Gamma}{E_d (\Gamma + iE_d)^3} + \frac{i\Gamma}{E_d^2 (\Gamma + iE_d)^2} \right] \right] \right]$$

$$\times \psi \left[\frac{1}{2} + \frac{\Gamma + iE_d}{2\pi T_{c0}} \right]. \quad (25)$$

In writing Eqs. (24) and (25) we have used Eqs. (14), (11), and (A6). Equations (21)–(23) give

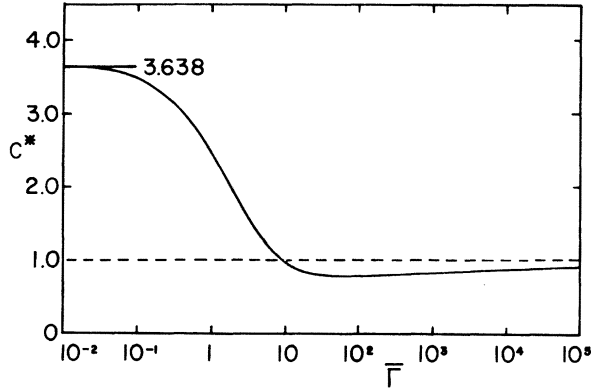


FIG. 2. $\bar{\Gamma}$ dependence of the initial slope of the normalized jump in specific heat vs the normalized transition temperature curve. The quantity C^* is defined in Eq. (33).

$$\frac{\Delta C/T_c}{\Delta C_0/T_{c0}} = 1 + n_i(b_{01} + b_1) + \dots \quad (26)$$

Thus $b_{01} + b_1$ represents the initial slope of the $(\Delta C/T_c)/(\Delta C_0/T_{c0})$ -vs- n_i curve. For $|(\Gamma + iE_d)/2\pi T_{c0}| \gg 1$, Eqs. (24)–(26) give

$$\frac{\Delta C/T_c}{\Delta C_0/T_{c0}} = 1 + n_i \frac{\Gamma}{\pi N_0(\Gamma^2 + E_d^2)} + \dots \quad (27)$$

For $E_d = 0$, Eq. (27) agrees with Eq. (4.21) of Ref. 8. For $|(\Gamma + iE_d)/2\pi T_{c0}| \ll 1$, Eqs. (24)–(26) give

$$\frac{\Delta C/T_c}{\Delta C_0/T_{c0}} = 1 - n_i \frac{32\Gamma}{\pi N_0(2\pi T_{c0})^2} \left[\lambda(3) - \frac{3\lambda(5)}{8\lambda(3)} - \left[6\lambda(4) - \frac{2\lambda(6)}{\lambda(3)} \right] \frac{\Gamma}{2\pi T_{c0}} \right] + \dots \quad (28)$$

Comparing Eqs. (27) and (28), one notes that the initial slope of the $\Delta C/T_c$ -vs- n_i curve is positive in the first case but is negative in the second case.

It is also interesting to study the initial slope of the $\Delta C/\Delta C_0$ -vs- T_c/T_{c0} curve defined by

$$C^* = \lim_{n_i \rightarrow 0} \frac{(\Delta C - \Delta C_0)/n_i \Delta C_0}{(T_c - T_{c0})/n_i T_{c0}} \quad (29)$$

Using Eqs. (13), (26), and (29), we obtain

$$C^* = 1 - (b_{01} + b_1)/b_0 \quad (30)$$

For $|(\Gamma + iE_d)/2\pi T_{c0}| \gg 1$, Eqs. (29), (15), and (27) yield

$$C^* = 1 - \left[\ln \left[4\gamma_e \frac{(E_d^2 + \Gamma^2)^{1/2}}{2\pi T_{c0}} \right] - \frac{\Gamma}{E_d} \arctan \frac{E_d}{\Gamma} \right]^{-1} + \dots \quad (31)$$

In this case C^* is less than 1. For $|(\Gamma + iE_d)/2\pi T_{c0}| \ll 1$, Eqs. (29), (16), and (28) give

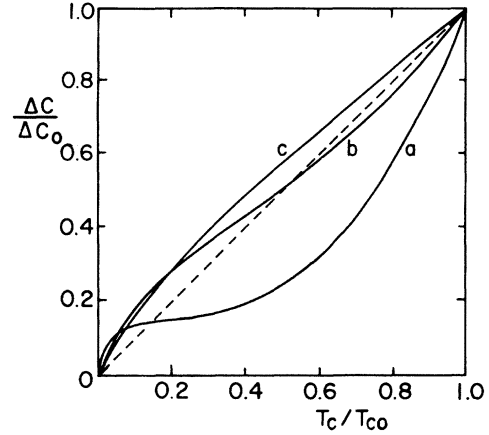


FIG. 3. Normalized jump in specific heat at T_c vs T_c/T_{c0} for $\bar{\Gamma} = 1.0$ (curve *a*), 5.0 (curve *b*), and 25.0 (curve *c*). The dashed line denotes the BCS result.

$$C^* = 5 - \frac{3\lambda(5)}{2[\lambda(3)]^2} - \left[\frac{8\lambda(4)}{\lambda(3)} - \frac{8\lambda(6)}{[\lambda(3)]^2} + \frac{6\lambda(4)\lambda(5)}{[\lambda(3)]^3} \right] \frac{\Gamma}{2\pi T_{c0}} + O \left[\frac{E_d^2 + \Gamma^2}{T_{c0}^2} \right] \quad (32)$$

The maximum value of C^* given by above equation is 3.638. It is the highest value reported in the literature for the impurity problem (see Table I). The detailed dependence of C^* on $\Gamma/\Delta_0(0)$ is shown in Fig. 2.

The variation of $\Delta C/\Delta C_0$ with T_c/T_{c0} is computed us-

TABLE I. Maximum value of the initial slope C^* .

Model	C^*
BCS Value	1.000
Abrikosov-Gor'kov ^a	1.436
Shiba-Rusinov ^b	2.219
MullerHartmann-Zittartz ^c	2.481
(Kondo effect)	
Present	3.638

^aReference 13.

^bReferences 10 and 14.

^cReference 15.

ing Eqs. (21) and (10)–(12). For the symmetric case ($E_d=0$), $\Delta C/\Delta C_0$ -vs- T_c/T_{c0} curves for $\Gamma/\Delta_0(0)=1.0, 5.0$, and 25.0 are shown in Fig. 3.

III. DENSITY OF STATES AND TUNNELING CONDUCTANCE

In this section we consider the electron-tunneling properties. The normalized electronic density of states is given by

$$\frac{N(\omega)}{N_0} = \text{Re} \left[\frac{U}{(U^2 - 1)^{1/2}} \right], \tag{33}$$

where the equation for the function U is obtained from Eq. (2) by replacing U_n with $-iU$ and ω_n with $-i\omega$ (with ω as the frequency). The changes in the density of states and the impurity band with a change in Γ are shown in Figs. 4–7, where we have taken zero temperature and $\Gamma/\Delta(0)=0.2, 1.0, 5.0$, and 25.0 , respectively. In each figure, various curves correspond to different values of the normalized impurity concentration \bar{n}_i . Here $\Delta(0)$ is the zero-temperature order parameter of the alloy and $\bar{n}_i = n_i/\pi N_0 \Delta(0)$. We have taken $E_d=0$. We note a systematic increase in the first gap as Γ is increased. We also

note the decrease in the first gap with an increase in \bar{n}_i . However, as is already known in the literature, there is no gapless superconductivity in the present model.

The bound states are usually searched by doing a tunneling experiment. For a N - I - S tunnel junction (N, I , and S stand for the normal metal, insulator, and the superconductor containing impurities), the normalized tunneling conductance is given by

$$g(V) = \frac{(dI/dV)_{NS}}{(dI/dV)_{NN}} = \frac{1}{4T} \int_{-\infty}^{\infty} d\omega \frac{N(\omega)}{N_0} \text{sech}^2 \left[\frac{\omega + V}{2T} \right]. \tag{34}$$

At a finite temperature, $N(\omega)/N_0$ vs ω/Δ is obtained as noted earlier. In order to get $g(V)$, the order parameter Δ at various temperatures and impurity concentrations is required. At a nonzero temperature we compute Δ using Eqs. (4) and (2). At $T=0$, we use Eq. (2) and

$$\ln \left[\frac{\Delta(0)}{\Delta_0(0)} \right] = \int_0^{\infty} d \left[\frac{\omega_n}{\Delta(0)} \right] \left[\frac{1}{(U_n^2 + 1)^{1/2}} - \frac{1}{\{[\omega_n/\Delta(0)]^2 + 1\}^{1/2}} \right]. \tag{35}$$

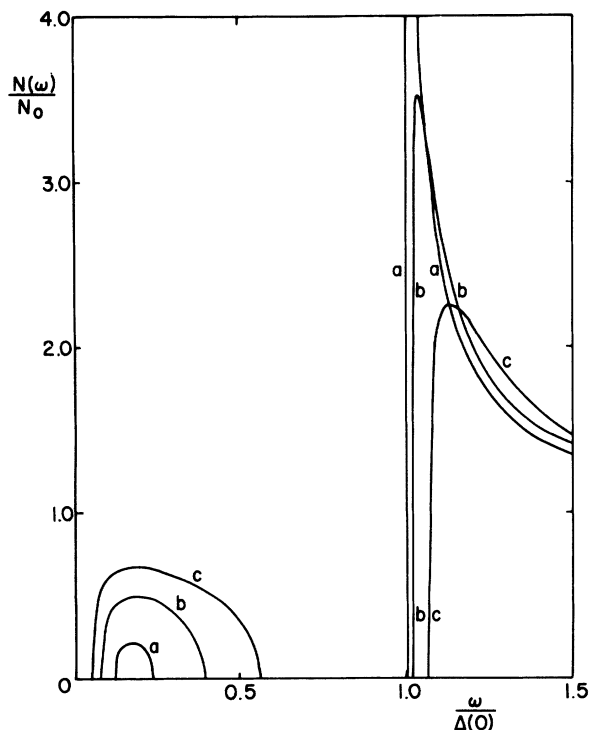


FIG. 4. Normalized electronic density of states $N(\omega)/N_0$ vs the normalized quasiparticle energy $\omega/\Delta(0)$ for $\bar{\Gamma}=0.2$ and $\bar{n}_i=0.1$ (curve a), 0.5 (curve b), and 1.0 (curve c). Here $\Delta(0)$ is the zero-temperature order parameter of the alloy. We have taken $T=0$.

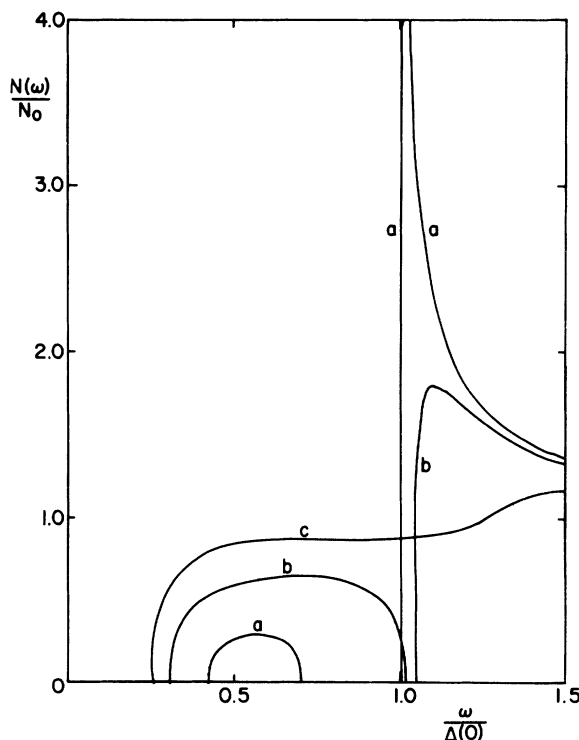


FIG. 5. $N(\omega)/N_0$ vs $\omega/\Delta(0)$ for $\bar{\Gamma}=1.0$. The values of \bar{n}_i for various curves are same as in Fig. 4.

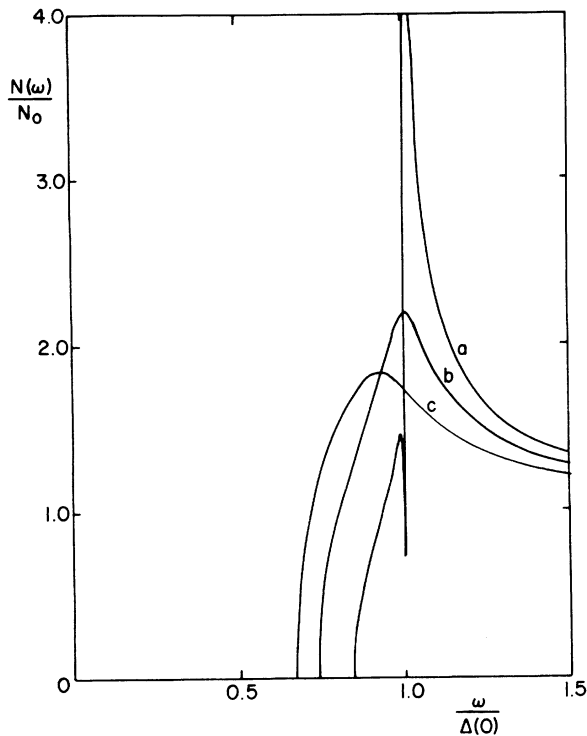


FIG. 6. $N(\omega)/N_0$ vs $\omega/\Delta(0)$ for $\bar{\Gamma}=5.0$. The values of \bar{n}_i for various curves are same as in Fig. 4.

Our results for $g(V)$ versus normalized voltage $V/\Delta(T)$ for $\Gamma/\Delta(0)=1.0$, $\bar{n}_i=0.1$, and $T/T_{c0}=0.0, 0.05, 0.1, 0.2$, and 0.4 are shown in Fig. 8. We can see how the structure is washed out as the temperature is raised. The value of Γ for the materials investigated so far is considered to be fairly large. The tunneling conductance curves for a much larger value of Γ , i.e., $\Gamma/\Delta(0)=25.0$, are shown in Fig. 9. We have taken $\bar{n}_i=0.01$ and $T/T_{c0}=0.0, 0.0005$, and 0.002 . Here the second gap is resolvable in curve *b*. We emphasize that the ultra-low-temperature measurement is essential for the search of the bound states in the present system with large Γ . Recently, a temperature of 200 mK was used by Bauriedl, Ziemann, and Buckel¹⁶ to observe impurity bands in superconductors with magnetic impurities.

IV. SUMMARY AND DISCUSSIONS

Using the Anderson model in the nonmagnetic limit, we have calculated some properties of the superconducting virtual-bound-state alloys. The general expressions for the impurity dependence of the transition temperature T_c and the jump in specific heat at T_c , ΔC , have been given. Special attention is given to the systematic variation of these quantities with respect to the resonance width Γ . As for the numerical results, we have only shown those for the symmetric case ($E_d=0$) in this paper. For smaller values of Γ , say $\Gamma \lesssim T_c$, we have found interesting behavior. The maximum value of the initial slope of the ΔC -vs- T_c curve is the highest reported in the literature for the impurity problem. Our results may help recognize materials with $\Gamma \sim T_c$. We have also calculated the electronic density of

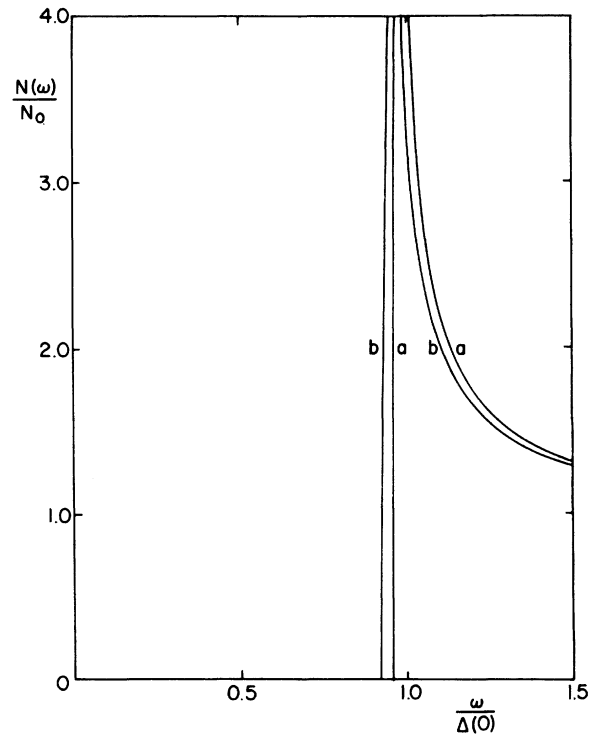


FIG. 7. $N(\omega)/N_0$ vs $\omega/\Delta(0)$ for $\bar{\Gamma}=25.0$ and $\bar{n}_i=0.5$ (curve *a*), 1.0 (curve *b*).

states for various values of Γ . The tunneling conductance and its temperature dependence have been shown.

In most of the earlier studies, Γ was taken larger than ω_D . With this assumption, Kaiser⁹ employed the approxi-

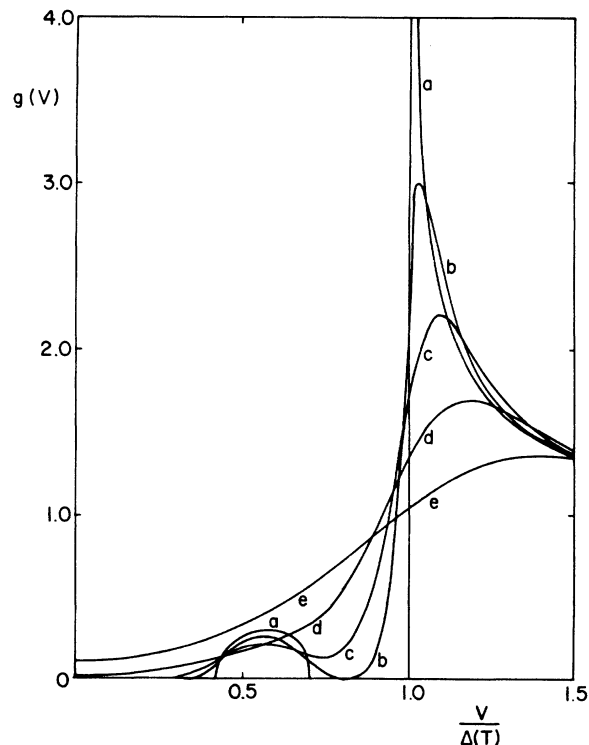


FIG. 8. Normalized tunneling conductance $g(V)$ vs normalized voltage $V/\Delta(T)$ for $\Gamma=1.0$, $\bar{n}_i=0.1$, and $T/T_{c0}=0.0$ (curve *a*), 0.05 (curve *b*), 0.1 (curve *c*), 0.2 (curve *d*), and 0.4 (curve *e*).

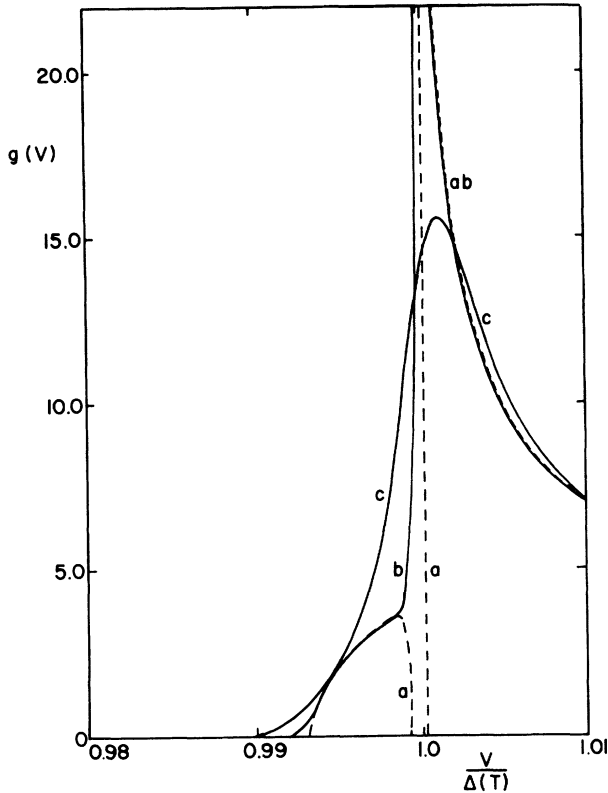


FIG. 9. $g(V)$ vs $V/\Delta(T)$ for $\bar{\Gamma}=25.0$, $\bar{n}_i=0.01$, and $T/T_{c0}=0.0$ (curve a), 0.0005 (curve b), and 0.002 (curve c).

mate form for the denominator in the right-hand side of Eq. (2) and used the cutoff ω_D in Eq. (4) to guarantee the convergence. Such an approach was also taken in other studies.^{10,17} In this paper we have used the exact form for Eq. (2) and assumed $\Gamma < \omega_D$ implicitly. One should be careful in the discussion of large- Γ behavior. In case of $\Gamma > \omega_D$, we can reproduce Kaiser's result by replacing the divergent term $\ln(E_d^2 + \Gamma^2)^{1/2}$ by $\ln\omega_D$, and so on.

In the present paper we have considered the nonmagnetic limit, i.e., $U=0$. When $U \neq 0$ but is still small as the

system is nonmagnetic, we should also consider the induced pairing of the d states represented by the parameter Δ_d .^{9,10} In this case the U_n equation is modified, and we cannot get simple forms for $B_0(n_i, T)$ and $B_1(n_i, T)$ as in Eqs. (10) and (11). However, we have verified that the qualitative nature of the results presented here remain unchanged.

Now we comment on the experimental search for the bound states in superconductors with nonmagnetic Anderson impurities. For this purpose, low- Γ materials are needed. Our ΔC -vs- T_c curve may help identify such alloys. For Al-Mn, as correctly reasoned by Terris and Ginsberg,¹ Γ/T_c is too large. For a tunneling search of the bound states in alloys with relatively large Γ , an ultra-low-temperature experiment is desirable.

ACKNOWLEDGMENTS

We thank Professor D. M. Ginsberg for sending us his paper prior to publication. This work is supported in part by the Natural Sciences and Engineering Research Council of Canada.

APPENDIX: DERIVATION OF EQS. (10) AND (11)

Using Eqs. (6) and (9), we get

$$B_0(n_i, T) = 2\pi T \sum_{n=0}^{\infty} \frac{\gamma}{\omega_n [A + \gamma]}, \quad (\text{A1})$$

$$B_1(n_i, T) = (2\pi T)^3 \sum_{n=0}^{\infty} \frac{A^2 [2\gamma\Gamma\omega_n + A(A + \gamma)]}{\omega_n^3 (A + \gamma)^4}, \quad (\text{A2})$$

where

$$A = E_d^2 + (\Gamma + \omega_n)^2. \quad (\text{A3})$$

Resolving into partial fractions and performing the summations, Eqs. (A1) and (A2) give

$$B_0(n_i, T) = \frac{\gamma}{\Gamma^2 + \alpha^2} \left\{ \text{Re} \left[\psi \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] \right] - \psi\left(\frac{1}{2}\right) - \frac{\Gamma}{\alpha} \text{Im} \left[\psi \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] \right] \right\}, \quad (\text{A4})$$

$$B_1(n_i, T) = -\frac{D_1}{2} \psi^{(2)}\left(\frac{1}{2}\right) + D_2 (2\pi T) \psi^{(1)}\left(\frac{1}{2}\right)$$

$$+ \text{Re} \left\{ \frac{D_3}{12\pi T} \psi^{(3)} \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] - \frac{D_4}{2} \psi^{(2)} \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] + D_5 (2\pi T) \psi^{(1)} \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] \right. \\ \left. - D_6 (2\pi T)^2 \left[\psi \left[\frac{1}{2} + \frac{\Gamma + i\alpha}{2\pi T} \right] - \psi\left(\frac{1}{2}\right) \right] \right\} \quad (\text{A5})$$

with

$$\begin{aligned}
D_1 &= \left[\frac{\Gamma^2 + \alpha^2 - \gamma}{\Gamma^2 + \alpha^2} \right]^3, \quad D_2 = \frac{8\gamma\Gamma(\Gamma^2 + \alpha^2 - \gamma)^2}{(\Gamma^2 + \alpha^2)^4}, \quad D_3 = \frac{\gamma^3\Gamma}{4\alpha^4(\Gamma + i\alpha)^2}, \\
D_4 &= \frac{i\gamma^2}{4\alpha^5(\Gamma + i\alpha)^2} \left[2\Gamma \left[2\alpha^2 - \gamma - \frac{i\gamma\alpha}{\Gamma + i\alpha} \right] - \frac{\gamma\alpha^2}{\Gamma + i\alpha} \right], \\
D_5 &= \frac{\gamma}{8\alpha^6(\Gamma + i\alpha)^2} \left[-\Gamma \left[8\alpha^4 - 12\gamma\alpha^2 + 5\gamma^2 - \frac{8i\gamma\alpha(2\alpha^2 - \gamma)}{\Gamma + i\alpha} - \frac{6\gamma^2\alpha^2}{(\Gamma + i\alpha)^2} \right] + 3\gamma\alpha^2 \left[\frac{4\alpha^2 - \gamma}{\Gamma + i\alpha} - \frac{2i\gamma\alpha}{(\Gamma + i\alpha)^2} \right] \right], \\
D_6 &= \frac{i\gamma}{8\alpha^7(\Gamma + i\alpha)^2} \left\{ \Gamma \left[(8\alpha^4 - 12\gamma\alpha^2 + 5\gamma^2) \left[1 + \frac{2i\alpha}{\Gamma + i\alpha} \right] + \frac{12\gamma\alpha^2(2\alpha^2 - \gamma)}{(\Gamma + i\alpha)^2} - \frac{8i\gamma^2\alpha^3}{(\Gamma + i\alpha)^3} \right] \right. \\
&\quad \left. + 3\alpha^2 \left[\frac{8\alpha^4 - 4\gamma\alpha^2 + \gamma^2}{\Gamma + i\alpha} - \frac{3i\gamma\alpha(4\alpha^2 - \gamma)}{(\Gamma + i\alpha)^2} - \frac{4\gamma^2\alpha^2}{(\Gamma + i\alpha)^3} \right] \right\}.
\end{aligned} \tag{A6}$$

In the equations above $\alpha = (E_d^2 + \gamma)^{1/2}$, $\psi^{(n)}(z)$ are polygamma functions,¹² and Re (Im) stands for the real (imaginary) part of the functions.

*On leave of absence from Department of Physics, Tohoku University, Sendai 980, Japan.

¹B. D. Terris and D. M. Ginsberg, Phys. Rev. B **27**, 1619 (1983).

²M. M. Salomaa and R. M. Nieminen, Z. Phys. B **35**, 15 (1979).

³P. W. Anderson, Phys. Rev. **124**, 41 (1961).

⁴A. D. S. Nagi and U. N. Upadhyaya, J. Phys. F **6**, 2353 (1976).

⁵K. Machida and F. Shibata, Prog. Theor. Phys. **47**, 1817 (1972).

⁶M. J. Zuckermann, Phys. Rev. **140**, A899 (1965).

⁷C. F. Ratto and A. Blandin, Phys. Rev. **156**, 513 (1967).

⁸M. Kiwi and M. J. Zuckermann, Phys. Rev. **164**, 548 (1967).

⁹A. B. Kaiser, J. Phys. C **3**, 410 (1970).

¹⁰H. Shiba, Prog. Theor. Phys. **40**, 435 (1968); **50**, 50 (1973).

¹¹Y. Okabe and A. D. S. Nagi, Solid State Commun. **46**, 639

(1983).

¹²P. J. Davis, in *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), pp. 253–294.

¹³A. A. Abrikosov and L. P. Gorkov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys.—JETP **12**, 1243 (1961)].

¹⁴A. I. Rusinov, Zh. Eksp. Teor. Fiz. **56**, 2047 (1969) [Sov. Phys.—JETP **29**, 1101 (1969)].

¹⁵E. Muller-Hartmann and J. Zittartz, Solid State Commun. **11**, 401 (1972).

¹⁶W. Bauriedl, P. Ziemann, and W. Buckel, Phys. Rev. Lett. **47**, 1163 (1981).

¹⁷G. B. Arnold, Phys. Rev. B **10**, 105 (1974).