PHYSICAL REVIEW B VOLUME 39, NUMBER 16 1 JUNE 1989

Thermodynamic properties of impure anisotropic quasi-one-dimensional superconductors

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(Received 22 December 1988)

The effects of nonmagnetic impurities on quasi-one-dimensional superconductors with anisotropic order parameters are studied in the framework of mean-field theory. We calculate the temperature dependence of the magnetic susceptibility and the specific heat and examine the low-temperature properties in terms of the density of states. The behavior of these thermodynamic quantities shows how the superconducting state is destroyed as the impurity concentration increases.

I. INTRODUCTION

Recently there have been extensive studies of the superconductivity in quasi-one-dimensional conductors.[1,2] Since the anisotropy of the electrical conductivity is large, remarkable differences between this superconducting (SC) state and the usual BCS state are found. Assuming that the electron-phonon interaction on individual chains is the microscopic origin of the SC state, one finds a large anisotropy of the coherence length and a nonzero gap parameter on the whole Fermi surface. On the other hand, another type of SC state has been proposed noting that the phase transition from the SC state into a spin-density-wave state takes place easily by varying the pressure or the magnetic field. In fact, recent NMR experiments on $(TMTSF)_2$ X compounds (where TMTSF represents tetramethyltetraselenafulvalene) indicate that the temperature dependence of the NMR relaxation rate at low temperature has a power-law behavior instead of the usual exponential decay of standard BCS theory.[3] This fact has been interpreted assuming an anisotropic superconducting (ASC) state with a line of zeros of the gap parameter on the Fermi surface.[4,5] As a model system which represents such a state, one can consider an array of one-dimensional (1D) chains with an attractive interaction between chains.[6,4] It has been proposed that the repulsive intrachain interaction gives rise to such an attraction.[7]

The existence of the ASC state is not yet fully established since precise measurements at very low temperatures are needed. The nature of the superconducting state can also be examined by adding nonmagnetic impurities. It is known that the ASC state vanishes above a critical concentration of the impurity[8] while the usual SC transition temperature is independent of the concentration. From the study in the clean case,[4] the thermodynamic properties of the ASC state are expected to be qualitatively similar to those of heavy-fermion systems. However, a more quantitative understanding of the ASC state in quasi-one-dimensional conductors is necessary in order to determine experimentally whether such a state is responsible for the superconductivity of these compounds. In the present paper, we examine the effect of nonmagnetic impurities on the temperature dependence of the magnetic susceptibility and the specific heat. We relate these quantities to the quasiparticle density of states in the superconducting state.

In Sec. II, the general formulation of the problem is given within the mean-field approximation and the SC order parameter is calculated. The density of states is calculated from the single-particle Green's function in Sec. III. We study the magnetic susceptibility in Sec. IV and the specific heat in Sec. V. Section VI is devoted to a discussion of our results.

II. FORMULATION

We consider the Hamiltonian

$$H=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}C^{\dagger}_{\mathbf{k},\sigma}C_{\mathbf{k},\sigma}-\sum_{\mathbf{k}}\Delta_{\mathbf{k}}(C^{\dagger}_{\mathbf{k}\uparrow}C^{\dagger}_{-\mathbf{k}\downarrow}+\text{h.c.})+N\Delta^2/g +(V_0/N)\sum_{\mathbf{k},\mathbf{k}',\sigma}\sum_{j}C^{\dagger}_{\mathbf{k},\sigma}C_{\mathbf{k}',\sigma}\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j]\ . \tag{2.1}$$

The first-term is the kinetic energy with $\varepsilon_{\mathbf{k}}=v_F(|k_x|-k_F)-2t_b\cos k_y$, where v_F and k_F are the Fermi velocity and momentum of the 1D chain and t_b is the hopping energy between chains. We consider the case where the hopping energy along the z axis is much smaller than t_b and therefore discard this degree of freedom. In the second and third term of (2.1), we consider only the attractive interaction between chains and treat it in the mean-field approximation. In the case of singlet pairing, one obtains d-wave superconductivity with an order parameter Δ_k given by

$$\Delta_{\mathbf{k}}=\Delta\cos k_y,\quad \Delta=\frac{g}{N}\sum_{\mathbf{k}}(\cos k_y)\langle C_{-\mathbf{k}\downarrow}C_{\mathbf{k}\uparrow}\rangle_H\ , \tag{2.2}$$

where g is the coupling constant. We assume that Δ is real. Equation (2.2) is a simplified order parameter compared to that of Ref. 4 which also takes into account the on-site repulsion. However, both cases give essentially the same result for properties arising from the gapless regions on the Fermi surface. The last term of Eq. (2.1) denotes the coupling with the impurities where V_0 is the magnitude of the impurity potential and N is the total number of lattice sites. The single-particle electron Green's function is defined by

$$G(i\omega_n,\mathbf{k}) = -\tfrac{1}{2}\int_{-1/T}^{1/T} d\tau \langle T_\tau \Psi_{\mathbf{k}}(\tau)\Psi_{\mathbf{k}}^\dagger(0)\rangle_H \times \exp(i\omega_n\tau) , \quad (2.3)$$

where $\Psi_{\mathbf{k}}^\dagger = (C_{\mathbf{k}\uparrow}^\dagger, C_{-\mathbf{k}\downarrow})$ and ω_n is the Matsubara frequency. T_τ is the ordering operator for the imaginary time. By treating the last term of Eq. (2.1) within the self-consistent Born approximation, Eq. (2.3) is rewritten as[9]

$$G^{-1}(i\omega_n,\mathbf{k}) = i\omega_n - \varepsilon_{\mathbf{k}}\sigma_3 + \Delta_{\mathbf{k}}\sigma_1 - \Sigma(i\omega_n,\mathbf{k}) , \quad (2.4)$$

where σ_j $(j=1,2,3)$ are the Pauli matrices and the self-energy is given by

$$\Sigma(i\omega_n,\mathbf{k}) = \frac{n_i V_0^2}{N}\sum_{\mathbf{k}} \sigma_3 G(i\omega_n,\mathbf{k})\sigma_3 . \quad (2.5)$$

From Eqs. (2.4) and (2.5), one obtains

$$G(i\omega_n,\mathbf{k}) = -\frac{i\tilde{\omega}_n + \varepsilon_{\mathbf{k}}\sigma_3 - \Delta_{\mathbf{k}}\sigma_1}{\tilde{\omega}_n^2 + \varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} , \quad (2.6)$$

where

$$\tilde{\omega}_n = \omega_n + \frac{\tilde{\omega}_n}{2\tau}\left\langle \frac{1}{(\tilde{\omega}_n^2 + \Delta_{\mathbf{k}}^2)^{1/2}} \right\rangle , \quad (2.7)$$

$$\frac{1}{\tau} = 2\pi n_i V_0^2 N_0 / N . \quad (2.8)$$

In Eq. (2.8), $N_0 = Na/\pi v_F$ is the density of states per spin in the normal state, a is the lattice constant along the x axis, and $n_i = N_{\text{imp}}/N$ is the impurity concentration. Note that Eq. (2.5) renormalizes ω_n but does not renormalize $\Delta_{\mathbf{k}}$. In Eq. (2.7), $\langle \dots \rangle$ denotes the average over k_y, i.e., $\langle \dots \rangle = \pi^{-1}\int_0^\pi dk_y \dots$. We use k in place of k_y or $\mathbf{k}$ if there is no confusion. From Eqs. (2.2) and (2.6), the order parameter Δ is determined self-consistently by

$$\frac{1}{\lambda} = T\sum_{n=-\infty}^{\infty}\left\langle \int_{-\omega_D}^{\omega_D} d\varepsilon \frac{\cos^2 k}{\tilde{\omega}_n^2 + \varepsilon^2 + \Delta_k^2} \right\rangle , \quad (2.9)$$

where $\lambda = gN_0/N$ and ω_D is the cutoff energy. Equation (2.9) is rewritten as

$$\frac{1}{2}\ln\frac{T}{T_{c0}} = \pi T \sum_n \left\langle \frac{(\cos k)^2}{(\tilde{\omega}_n^2 + \Delta_k^2)^{1/2}} - \frac{\cos^2 k}{|\omega_n|} \right\rangle , \quad (2.10)$$

where

$$T_{c0} = (2e^\gamma/\pi)\omega_D \exp(-2/\lambda) .$$

By putting $\Delta = 0$ in Eq. (2.10), the equation for T_c is obtained as

$$\ln\frac{T_c}{T_{c0}} = \psi(\tfrac{1}{2}) - \psi(\tfrac{1}{2}+\alpha) , \quad (2.11)$$

where $\alpha = 1(4\pi\tau T_c)$. Equation (2.11) was obtained in Ref. 8 which treated the effect of nonmagnetic impurity on the several kinds of SC pairing states. The quantity α is the pair-breaking parameter which is half of that corresponding to the usual BCS state in the presence of magnetic impurities.[10] In Fig. 1, T_c is calculated as a function of $1/\tau$. The quantity T_c vanishes at $\tau = \tau_0$, where

$$1/(\tau_0 T_{c0}) = \pi/e^\gamma . \quad (2.12)$$

The asymptotic forms of Eq. (2.11) are given by

$$T_c/T_{c0} \simeq 1 - (\pi^2/8e^\gamma)\tau_0/\tau$$

for $\tau_0/\tau \ll 1$ and

$$T_c/T_{c0} \simeq (\tfrac{3}{2})^{1/2} e^{-\gamma} |\ln\tau/\tau_0|^{1/2}$$

for $\tau/\tau_0 \sim 1$, respectively. By using (2.10), Δ as a function of T/T_{c0} is calculated for some choices of τ_0/τ in Fig. 2. In the case of $T \sim T_c$, Δ is calculated as

$$\Delta/T_c \simeq (a/b)^{1/2}(1-T/T_c)^{1/2} , \quad (2.13)$$

where

$$a = \frac{1}{2}\left[1 - \alpha\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2}+\alpha)^2}\right] , \quad (2.14)$$

$$b = \frac{3}{128\pi^2}\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2}+\alpha)^3}\left[1 - \frac{2\alpha/3}{n+\frac{1}{2}+\alpha}\right] . \quad (2.15)$$

In order to examine Δ at low temperatures, Eq. (2.9) is rewritten as

$$\frac{1}{\lambda} - \int_0^{\omega_D} d\omega_n \left\langle \frac{\cos^2 k}{(\tilde{\omega}_n^2 + \Delta_k^2)^{1/2}} \right\rangle = -2\int_0^\infty d\omega \,\mathrm{Im}\left\langle \frac{\cos^2 k}{(-\omega^2 + \Delta_k^2)^{1/2}} \right\rangle \frac{1}{\exp[\omega/T]+1} . \quad (2.16)$$

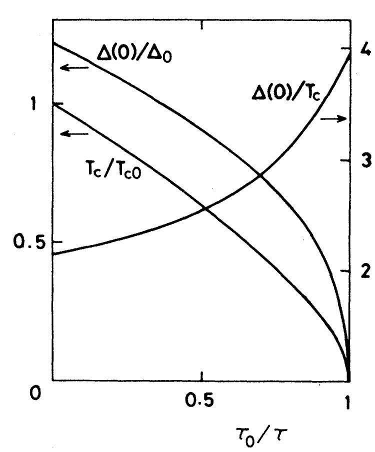

FIG. 1. Normalized T_c, $\Delta(0)$, and $\Delta(0)/T_c$ as a function of τ_0/τ. The ratio $\Delta(0)/T_c$ increases as τ_0/τ increases.

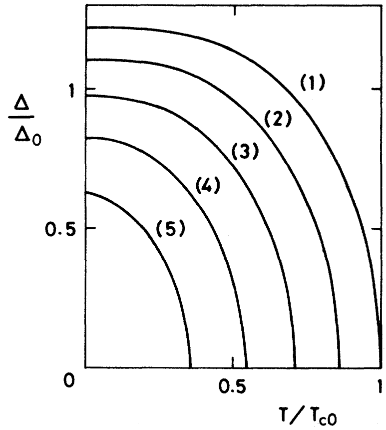

FIG. 2. Normalized order parameter Δ/Δ_0 as a function of T/T_c, with $\tau_0/\tau=0$ (1), 0.2 (2), 0.4 (3), 0.6 (4), and 0.8 (5).

In Eq. (2.16), $\tilde{\omega}$ is the analytically continued value of $i\tilde{\omega}_n$ which is obtained from (2.7) with $i\omega_n=\omega+i0$. We define $\Delta(0)$ as Δ at $T=0$ which is obtained by putting the right-hand side of (2.16) zero. When $\tau^{-1}=0$, one obtains $\Delta(0)=2e^{-1/2}\Delta_0$, where $\Delta_0=2\omega_D\exp(-2/\lambda)$. At low temperatures, (2.16) is calculated as

$$\Delta/\Delta(0)\simeq 1-3\zeta(3)(T/\Delta)^3 \quad (\tau^{-1}=0)\,, \tag{2.17}$$

$$\Delta/\Delta(0)\simeq 1-c(T/\Delta)^2 \quad (\tau^{-1}\neq 0)\,, \tag{2.18}$$

where

$$c=\frac{(\pi^2/6)x_1y_0\left\langle \dfrac{\Delta_k^2}{(y_0^2+\Delta_k^2)^{3/2}}\right\rangle}{\displaystyle\int_0^\infty d\omega_n\left\langle\frac{\Delta_k^2\cos^2k}{(\tilde{\omega}_n^2+\Delta_k^2)^{3/2}}\right\rangle}\,. \tag{2.19}$$

In Eq. (2.18), we used the fact that $\tilde{\omega}\simeq x_1\omega+iy_0$ for the small ω where x_1 and y_0 are calculated in Sec. III. In Fig. 1, $\Delta(0)/\Delta_0$ is shown as a function of τ_0/τ where the asymptotic behavior is given by $\Delta/\Delta(0)\simeq 1-0.52/\Delta\tau$ and $|(\frac{12}{5})\ln\tau_0/\tau|^{1/2}$ for $\tau_0/\tau\ll 1$ and ~ 1, respectively. The quantity $\Delta(0)/T_c$ is also shown in Fig. 1 where one finds $\Delta(0)/T_c=2\pi/e^{\gamma+1/2}$ and $\pi(\frac{8}{5})^{1/2}$ for $\tau_0/\tau=0$ and 1, respectively.

III. DENSITY OF STATES

By use of the Green's function (2.6), the electronic density of states normalized by N_0 is given by

$$D(\omega)=\frac{-1}{2\pi N_0}\sum_k \mathrm{Im}\mathrm{Tr}G^R(\omega,k)$$
$$=\mathrm{Im}\left\langle\frac{\tilde{\omega}}{(-\tilde{\omega}^2+\Delta_k^2)^{1/2}}\right\rangle\Bigg|_{i\omega_n=\omega+i0}\,. \tag{3.1}$$

The quantity $\tilde{\omega}$ is the analytically continued value obtained from

$$\tilde{\omega}=\omega+\frac{1}{2\tau}\left\langle\frac{\tilde{\omega}}{-\tilde{\omega}^2+\Delta_k^2)^{1/2}}\right\rangle\,. \tag{3.2}$$

The branch cut of the square root is chosen so as to obtain a positive value for the imaginary part of $\tilde{\omega}$. By writing $\tilde{\omega}=\omega_1+i\omega_2$, where ω_1 and ω_2 are real, Eq. (3.2) is rewritten as

$$\omega_1=\omega+\omega_1I_+-\omega_2I_-\,,$$
$$\omega_2=\omega_1I_-+\omega_2I_+\,, \tag{3.3}$$

where $I_\pm=(8^{1/2}\tau)^{-1}\langle r^{-1}(r\pm X)^{1/2}\rangle$, $r^2=X^2+4\omega_1^2\omega_2^2$, and $X=-\omega_1^2+\omega_2^2+\Delta_k^2$. For small ω, Eq. (3.3) is calculated as

$$\tilde{\omega}=\omega x_1+i(y_0+\omega^2y_2)+\cdots\,, \tag{3.4}$$

where y_0, x_1, and y_2 are given by

$$1=\frac{1}{2\tau}\left\langle\frac{1}{X_0^{1/2}}\right\rangle\,, \tag{3.5}$$

$$x_1=\frac{1}{1-\langle\Delta_k^2/X_0^{3/2}\rangle/2\tau}\,, \tag{3.6}$$

$$y_2=\frac{x_1^2y_0\langle(3\Delta_k^2+y_0^2)/X_0^{5/2}\rangle}{4\tau(1-\langle\Delta_k^2/X_0^{3/2}\rangle/2\tau)}\,, \tag{3.7}$$

and $X_0=y_0^2+\Delta_k^2$. For both large and small τ Eq. (3.5) becomes

$$y_0=4\Delta\exp(-\pi\tau\Delta) \quad (\tau\Delta\gg 1)\,,$$
$$y_0=(2\tau)^{-1}[1-(\Delta\tau)^2] \quad (\tau\Delta\ll 1)\,. \tag{3.8}$$

The asymptotic form of x_1 and y_2 for small $1/\tau$ is

$$x_1\simeq\pi\tau\Delta \quad (y_0\ll\Delta)\,, \tag{3.9}$$

$$y_2\simeq(\tfrac{5}{6})(\pi\tau\Delta)^2/y_0 \quad (y_0\ll\Delta)\,. \tag{3.10}$$

By use of Eq. (3.2), Eq. (3.1) is rewritten as[10]

$$D(\omega)=2\tau\omega_2\,. \tag{3.11}$$

From Eqs. (3.3) and (3.11), $D(\omega)$ at $T=0$ can be calculated numerically, and the results are shown in Fig. 3 for

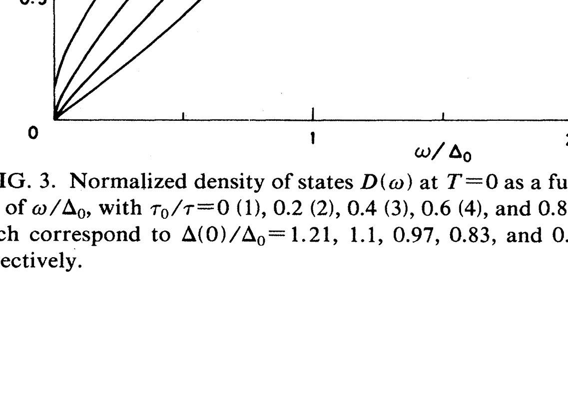

FIG. 3. Normalized density of states $D(\omega)$ at $T=0$ as a function of ω/Δ_0, with $\tau_0/\tau=0$ (1), 0.2 (2), 0.4 (3), 0.6 (4), and 0.8 (5) which correspond to $\Delta(0)/\Delta_0=1.21$, 1.1, 0.97, 0.83, and 0.63, respectively.

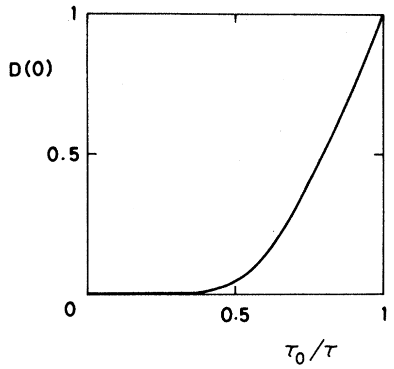

FIG. 4. Normalized density of states at the Fermi surface for $T=0$.

some choices of τ_0/τ. The quantity $D(\omega)$ at $\omega=0$ is finite for $\tau^{-1}\neq 0$. This can be seen noting

$$D(0)=2\tau y_0 , \tag{3.12}$$

and y_0 is always finite from Eq. (3.8). Numerical results for $D(0)$ are shown in Fig. 4 as a function τ_0/τ, and the limiting values are obtained as follows:

$$\begin{aligned} &D(0)\simeq 8\tau\Delta\exp[-\pi\tau\Delta] \quad (\tau_0/\tau \ll 1) , \\ &D(0)\simeq 1-(\tfrac{12}{5})\ln(\tau_0/\tau) \quad (\tau_0/\tau\sim 1) . \end{aligned} \tag{3.13}$$

For small $|\omega|$, $D(\omega)$ is

$$\begin{aligned} &D(\omega)\simeq|\omega|/\Delta \quad (\tau_0/\tau=0) , \\ &D(\omega)\simeq D(0)+2\tau y_2\omega^2 \quad (\tau_0/\tau\neq 0) . \end{aligned} \tag{3.14}$$

Since the expansion of $D(\omega)$ in terms of ω in the case of $\tau^{-1}\neq 0$ is valid for $|\omega|<y_0$, the ω^2 dependence is visible only for $\tau_0/\tau\sim 1$ in Fig. 3. The properties of the density of states studied here are similar to those of the polar state of heavy-fermion systems.[11,12] The ω dependence of $D(\omega)$ in the clean case and the finite value of $D(0)$ in the presence of impurities are the same except for numerical factors which depend on details of the Fermi surface. There is a difference of $D(\omega)$ around $|\omega|\simeq\Delta_0$ in the clean case because there is a logarithmic singularity in our case.

IV. MAGNETIC SUSCEPTIBILITY

We examine $\chi(T)$, the spin susceptibility which is normalized by its normal-state value. Since $\chi(T)$ corresponds to the density response function for a homogeneous magnetic field, the extension of Eq. (2.4) leads to

$$\chi(T)=\frac{T}{4H_0N_0}\sum_{k,n}\mathrm{Tr}[G(i\omega_n+H_0,k) - G(i\omega_n-H_0,k)]e^{i\omega_n\tau}|_{\tau\to+0,H_0\to 0} , \tag{4.1}$$

where we took $\mu_B=1$. By use of Eq. (2.7), (4.1) is rewritten as

$$\begin{aligned} \chi(T)&=\int d\varepsilon\frac{T}{2i}\sum_n\frac{\partial}{\partial\omega_n}\langle \mathrm{Tr}G(i\omega_n,k)\rangle \\ &=1-\pi T\sum_n\frac{\langle\Delta_k^2/(\tilde{\omega}_n^2+\Delta_k^2)^{3/2}\rangle}{1-(2\tau)^{-1}\langle\Delta_k^2/(\tilde{\omega}_n^2+\Delta_k^2)^{3/2}\rangle} , \end{aligned} \tag{4.2}$$

where the denominator of the second line shows the vertex correction by the impurity. In Fig. 5, $\chi(T)$ as a function of T is shown for fixed τ_0/τ.

The limiting values are calculated as follows. For $T\sim T_c$, Eqs. (2.13) and (4.2) lead to

$$\chi(T)\simeq 1-\frac{a\psi''(\frac{1}{2}+\alpha)}{32\pi^2 b}(1-T/T_c) , \tag{4.3}$$

where a and b are defined by Eqs. (2.14) and (2.15). For the study of $\chi(T)$ at low temperatures, we rewrite Eq. (4.2) by use of the density of states obtained in Sec. III,

$$\chi(T)=\int_0^\infty d\omega\, D(\omega)\frac{\partial}{\partial\omega}\frac{-2}{\exp(\omega/T)+1} , \tag{4.4}$$

where $D(\omega)$ is defined in Eq. (3.1). At low temperatures Eq. (4.4) becomes

$$\chi(T)\simeq(2\ln 2)T/\Delta \quad (\tau^{-1}=0) \tag{4.5}$$

$$\begin{aligned} \chi(T)&\simeq D(0)+\pi^2/6D''(0)T^2+\cdots \\ &=2\tau y_0+(2\pi^2/3)\tau y_2T^2+\cdots \quad (\tau^{-1}\neq 0) , \end{aligned} \tag{4.6}$$

where y_0 and y_2 are given by Eqs. (3.5) and (3.7). Note that Eq. (4.4) is the usual formula for a free-electron system in which one always obtains $\chi(0)=D(0)$. Since y_0 is small for small τ^{-1}, the T^2 dependence in Fig. 5 is visible for $\tau_0/\tau\sim 1$. In the case of $\tau^{-1}=0$, $\chi(T)$ shows a linear dependence on T and then is much larger than that of the usual BCS state which decreases exponentially.[13]

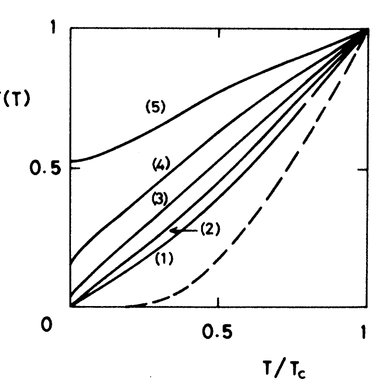

FIG. 5. Normalized magnetic susceptibility $\chi(T)$, with $\tau_0/\tau=0$ (1), 0.2 (2), 0.4 (3), 0.6 (4), and 0.8 (5). The dashed curve denotes the Yosida function corresponding to the usual BCS state which is shown for comparison.

V. SPECIFIC HEAT

We study the specific heat C_V by calculating the free energy. The quantity C_V is defined by

$$C_V=C_n(T)-T\frac{d^2}{dT^2}(\delta F) , \tag{5.1}$$

where δF is the excess free energy given by

$$\begin{aligned}\delta F/N_0&=\int_0^{\Delta^2}dz^2z^2\frac{d}{dz^2}[1/\lambda(z)]\\&=\Delta^2/\lambda-\int_0^{\Delta^2}dz^2T\sum_n\int_{-\omega_D}^{\omega_D}d\varepsilon\left\langle\frac{\cos^2k}{\tilde{\omega}_n^2+\varepsilon^2+z^2\cos^2k}\right\rangle .\end{aligned}\tag{5.2}$$

The quantity $C_n(T)$ denotes C_V in the normal state,

$$C_n(T)=(2\pi^2/3)N_0T . \tag{5.3}$$

First we examine the jump of the specific heat ΔC_V. By expanding (5.2) in terms of Δ and making use of (2.13), the quantity ΔC_V normalized by C_n is calculated as

$$\begin{aligned}\Delta C_V/C_n(T_c)=C_n^{-1}(T_c)[C_V-C_n(T_c)]_{T\to T_c-0}&=\frac{8\left[1-\alpha\sum_{n=0}^{\infty}(n+1/2+\alpha)^{-2}\right]^2}{\sum_{n=0}^{\infty}(n+\frac{1}{2}+\alpha)^{-3}[1-(2\alpha/3)/(n+\frac{1}{2}+\alpha)]}\\&=12\frac{[1-\alpha\psi'(\frac{1}{2}+\alpha)]^2}{-\frac{3}{4}\psi''(\frac{1}{2}+\alpha)-\frac{\alpha}{6}\psi'''(\frac{1}{2}+\alpha)} ,\end{aligned}\tag{5.4}$$

where $\alpha=1/4\pi\tau T_c$, and ψ',ψ'',ψ''' are polygamma functions. The asymptotic form of Eq. (5.4) is given by

$$\Delta C_V/C_n(T_c)\simeq(8/7)\zeta(3)(1-0.392\tau_0/\tau)$$

and $(\frac{24}{5})|\ln\tau_0/\tau|$ for $\tau_0/\tau\ll1$ and $\simeq1$, respectively. The numerical result of (5.4) is shown in Fig. 6. Results similar to Eq. (5.4) and Fig. 6 have already been found for isotropic superconductors with magnetic impurities[9,14] and for different types of p-wave superconductors.[11] The only difference is the numerical factor $\frac{3}{4}$ in the denominator of Eq. (5.4), which takes different values for different types of superconducting states, due to differences in the detailed structure of the gap parameter. For example, (5.4) in the case of $\tau^{-1}=0$ becomes $\frac{2}{3}$ of the usual BCS value while the corresponding value for the polar axial case is $\frac{5}{9}$.[11]

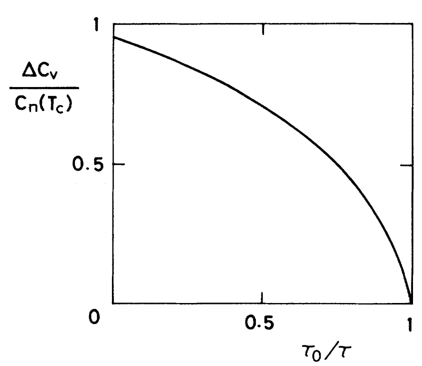

FIG. 6. Jump of the specific heat normalized to that of the normal state as a function of τ_0/τ.

Next we examine the temperature dependence of C_V numerically. We rewrite Eq. (5.1) as (see Appendix A)

$$C_V=C_n(T)+\frac{d}{dT}\delta E , \tag{5.5}$$

$$\delta E/N_0=-\frac{\Delta^2}{2}+2\pi T\sum_n\left[\left\langle\frac{\omega_n\tilde{\omega}_n}{(\omega_n^2+\Delta_k^2)^{1/2}}\right\rangle-|\omega_n|+\frac{1}{2}\left\langle\frac{\Delta_k^2}{(\tilde{\omega}_n^2+\Delta_k^2)^{1/2}}\right\rangle\right] . \tag{5.6}$$

From Eqs. (2.10) and (5.5), the quantity $C_V/C_n(T)$ is calculated and is shown in Fig. 7. When $1/\tau$ increases, the difference between C_V and $C_n(T)$ becomes small and Fig. 7 always satisfies the following condition:

$$\int_0^{T_c}dT[C_V/C_n(T)-1]=0 . \tag{5.7}$$

Now we study C_V at low temperatures. By use of the density of states Eq. (5.2) is rewritten as (see Appendix B)

$$\begin{aligned}\delta F/N_0=\frac{\Delta^2}{\lambda}&+2T\int_{|\omega|<\omega_D}d\omega\ln[1+\exp(-\omega/T)]\\&-2T\int_{|\omega|<((\omega_D^2+\Delta^2)^{1/2})}d\omega\, D(\omega)\times\ln[1+\exp(-\omega/T)] .\end{aligned}\tag{5.8}$$

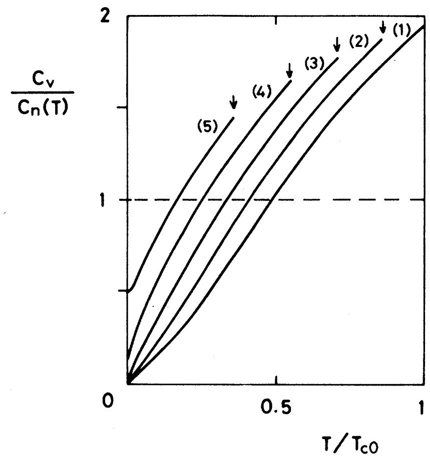

FIG. 7. Temperature dependence of the normalized specific heat with $\tau_0/\tau=0$ (1), 0.2 (2), 0.4 (3), 0.6 (4), and 0.8 (5). The arrow indicates the corresponding T_c. The dashed line is the normal-state specific heat.

The last two terms in Eq. (5.8) are the contribution of excited quasiparticles with density of states $D(\omega)$. This is due to the mean-field treatment of the attractive interaction in the second line of Eq. (2.1). Substituting Eq. (5.8) into Eq. (5.1) one obtains

$$\begin{aligned} C_V/N_0 &= A(T)\frac{d\Delta^2}{dT} + \int_{-\infty}^{\infty} d\omega\, \omega D(\omega)\frac{\partial}{\partial T}\left[\frac{1}{\exp(\omega/T)+1}\right] \\ &= A(T)\frac{d\Delta^2}{dT} + \frac{2\pi^2}{3}D(0)T + 18\zeta(3)D'(0)T^2 + \cdots , \end{aligned} \tag{5.9}$$

$$A(T) = \frac{1}{\lambda} - \frac{1}{2} + 2\int_{-\infty}^{\infty} d\omega \left[\frac{\partial}{\partial \Delta^2}D(\omega)\right] \times \frac{\omega}{\exp(\omega/T)+1} . \tag{5.10}$$

Equation (5.9) shows that the low-temperature behavior of C_V is determined not only by the density of states but also the temperature dependence of Δ. We therefore examine the quantity $A(0)$ which can be rewritten as

$$A(0) = -\tfrac{1}{2} + \int_0^{\infty} d\omega_n \left\langle \cos^2 k \frac{\tilde{\omega}_n(\tilde{\omega}_n - \omega_n) + \Delta_k^2}{(\tilde{\omega}_n^2 + \Delta_k^2)^{3/2}} \right\rangle . \tag{5.11}$$

In the case of the small τ^{-1}, we find

$$A(0) \simeq C_0/\tau\Delta \quad (1/\tau\Delta \ll 1) \tag{5.12}$$

with $C_0 \simeq 0.05$. Equation (5.12) shows that $A(0)=0$ at $\tau^{-1}=0$. Then the first term of Eq. (5.9) can be disregarded at low temperatures only for the clean system. From Eqs. (2.17), (2.18), (5.9), and (5.10), C_V at $T=0$ is calculated as

$$\left.\frac{C_V}{C_n(T)}\right|_{T=0} = D(0)(1-B) , \tag{5.13}$$

$$B = \frac{3A(0)c}{\pi^2 \tau y_0} . \tag{5.14}$$

For the case of $1/\tau\Delta \ll 1$, we find $B = 2\pi C_0 \simeq 0.3$. We obtain that B decreases with increasing $1/\tau$, actually $B \simeq 0.03$ for $\tau_0/\tau = 0.8$.

From Eq. (5.9), we find the low-temperature behavior as follows. In the clean case, C_V is calculated as

$$\frac{C_V}{C_n(T)} \simeq \frac{27\zeta(3)T}{\pi^2\Delta(0)} \quad (\tau^{-1}=0) . \tag{5.15}$$

In the dirty case the increase of C_V is proportional to T^2 although this is visible in Fig. 7 only for $\tau_0/\tau \sim 1$.

In the polar axial case[11] it has already been shown numerically that C_V at $T=0$ is finite for $1/\tau \neq 0$ but it is not yet clear if the value corresponding to Eq. (5.13) is simply given by $D(0)$ as in the case of $\chi(T)$ or has an extra factor like $(1-B)$. In the case of point zeros of the gap parameter, B has been claimed to be small,[15] however, to our knowledge there is no complete treatment of the $A(T)$ term in the heavy-fermion case.

VI. DISCUSSION

In the present paper, we have examined the effect of nonmagnetic impurities on quasi-one-dimensional superconductors with an anisotropic gap parameter, having line zeros on the Fermi surface. In this case, nonmagnetic impurities have a pair-breaking effect, similar to magnetic impurities in an isotropic superconductor. The effect of pair breaking was studied by examining the density of states, magnetic susceptibility, and specific heat. In all three quantities, rather strong impurity effects are found. The low-temperature properties can all be described in terms of the properties of the density of states around the Fermi surface. Our results for the specific heat should be rather straightforwardly comparable to experimental results. This could help to identify the superconductivity in $(TMTSF)_2X$ compounds with the d-type state proposed in Refs. 1–7.

Rather detailed experimental investigators of the thermodynamics of the superconducting transition in the organic compound $(TMTSF)_2ClO_4^-$ have been performed by Garoche and collaborators.[16,17] In that compound there is an order-disorder transition of the ClO_4^- anions at 24 K which can be completely or partially suppressed by more or less rapid cooling rates, leading to a certain degree of *nonmagnetic* disorder. Introducing disorder in this way leads to a decrease of T_c, i.e., the disorder has a pair-breaking effect. Experimental results for the normalized specific-heat jump[17] are shown in Fig. 8, together with our theoretical results. The agreement is very good, and this seems to provide some support for the d-wave nature of the superconducting state. There is, however, a

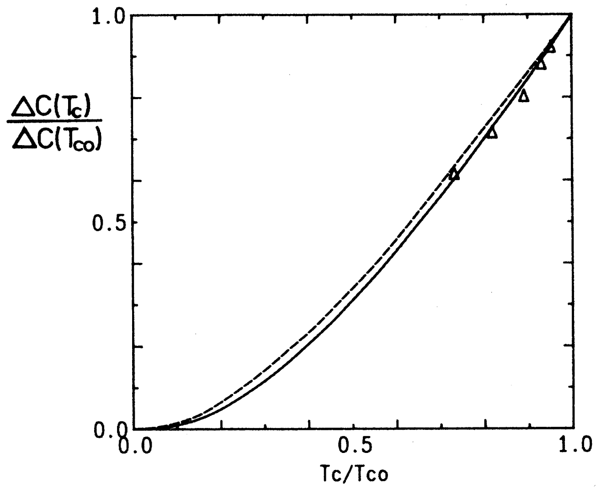

FIG. 8. Normalized specific-heat jump of an impure quasi-one-dimensional d-type superconductor as a function of reduced transition temperature (full line), where $\Delta C(T_c)$ denotes the ΔC_V at $T=T_c$. The dashed line is the corresponding result for an isotropic superconductor with magnetic impurities (Ref. 14), triangles are the data of Pesty *et al.* (Ref. 17).

problem with this interpretation: The theory predicts, for the pure case $\Delta C_V(T_c)/C_n(T_c)=0.95$,[6] whereas experimentally one finds a value of approximately 1.6. Whether this discrepancy is due to one-dimensional fluctuations,[18] strong-coupling effects, or some other source is not clear at present.

There is the following similarity between the present case and the polar case in heavy-fermion systems. In the clean case, the density of states around the Fermi surface is proportional to $|\omega|$ and then thermodynamic quantities show power-law behavior. In the presence of nonmagnetic impurities the density of states always remains finite and excited quasiparticles dominate the low-temperature thermodynamic properties. With decreasing impurity concentration $D(0)$ decreases exponentially. The difference of numerical factors which appears in the two cases comes from the dimensional dependence of the order parameter.

The density of states obtained here is also similar to that of d-wave superconductors on a two-dimensional square lattice.[10] Therefore the same temperature dependence can be expected for the thermodynamic quantities as the magnetic susceptibility and the specific heat although there will again be differences in numerical factors.

ACKNOWLEDGMENTS

We would like to thank D. Jérome for suggesting this problem and useful discussions. We are also grateful to F. Pesty for helpful discussions on the specific-heat data. This work was supported by the exchange program between Japan Society for the Promotion of Science and Centre National de la Recherche Scientifique.

APPENDIX A: PROOF OF EQ. (5.6)

From (5.1) and (5.2),

$$\delta E/N_0=-T^2\frac{d}{dT}(\delta F/N_0T)=\tfrac{1}{2}\Delta^2\ln\frac{T}{T_{c0}}-\tfrac{1}{2}\Delta^2+\int_0^{\Delta^2}dz^2\pi T\sum_n\omega_n\frac{d}{d\omega_n}\left[\left\langle\frac{\cos^2k}{(\tilde{\omega}_n^2+z^2\cos^2k)^{1/2}}\right\rangle-\frac{1}{2|\omega_n|}\right]. \tag{A1}$$

From (2.7), it is found that

$$\frac{d}{d\omega_n}\left\langle\frac{\cos^2k}{(\tilde{\omega}_n^2+\Delta_k^2)^{1/2}}\right\rangle=4\tau\frac{d\tilde{\omega}_n}{d\Delta^2}. \tag{A2}$$

Substituting (A2) into (A1) and making use of (2.7), one obtains (5.6).

APPENDIX B: PROOF OF EQ. (5.8)

Equation (5.2) is calculated as

$$\begin{aligned}\delta F/N_0&=\frac{\Delta^2}{\lambda}-\frac{\Delta^2}{2}\int_0^{\omega_D}\frac{d\varepsilon}{\varepsilon}\left[\tanh\frac{\varepsilon}{2T}\right]-\int_0^{\Delta^2}dz^2\pi T\sum_n\left[\left\langle\frac{\cos^2k}{(\tilde{\omega}_n^2+z_k^2)^{1/2}}\right\rangle-\frac{1}{2|\omega_n|}\right]\\&=\frac{\Delta^2}{\lambda}+\int_0^{\Delta^2}dz^2\int_{-\omega_D}^{\omega_D}d\omega\frac{1}{\exp(\omega/T)+1}\mathrm{Im}\left\langle\frac{\cos^2k}{(-\tilde{\omega}^2+z_k^2)^{1/2}}\right\rangle\\&=\frac{\Delta^2}{\lambda}+\int_0^{\Delta^2}dz^2\left[-T\ln(1+e^{-\omega/T})\mathrm{Im}\left\langle\frac{\cos^2k}{(-\tilde{\omega}^2+z_k^2)^{1/2}}\right\rangle\right]\Bigg|_{\omega=-\infty}^{\omega=\infty}\\&\quad+\int_{-\omega_D}^{\omega_D}d\omega\,T\ln(1+e^{-\omega/T})\frac{d}{d\omega}\mathrm{Im}\left\langle\frac{\cos^2k}{(-\tilde{\omega}^2+z_k^2)^{1/2}}\right\rangle,\end{aligned} \tag{B1}$$

where $z_k = z \cos k$. By use of (A2) with $i\omega_n = \omega$, (B1) is rewritten as

$$\delta F / N_0 = \frac{\Delta^2}{\lambda} - \langle \Delta_k^2 \rangle - 2T \int_{-\omega_D}^{\omega_D} d\omega \ln(1 + e^{-\omega/T})[D(\omega) - 1] , \tag{B2}$$

which leads to (5.8) in the case of $\Delta \ll \omega_D$.

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