Nonmagnetic impurity effects in MgB$_2$

Koichi Watanabe and Takafumi Kita

Division of Physics, Hokkaido University, Sapporo 060-0810, Japan
(Dated: December 28, 2021)

We study nonmagnetic impurity effects in MgB$_2$ using the quasiclassical equations of superconductivity for a weak-coupling two-band model. Parameters in the model are fixed so as to reproduce experiments on MgB$_2$ as closely as possible. The quasiparticle density of states and the specific heat are calculated for various values of the interband impurity scattering. The density of states changes gradually from a two-gap structure into the conventional single-gap structure as the interband scattering increases. It is found that the excitation threshold is not a monotonic function of the interband scattering. Calculated results for the specific heat are in good agreements with experiments on samples after irradiation.

PACS numbers: Valid PACS appear here

I. INTRODUCTION

Superconductivity in MgB$_2$ has attracted much attention since its discovery by Nagamatsu et al.\cite{Nagamatsu01} Besides its high transition temperature $T_c \cong 40K$ for a phonon-mediated pairing mechanism\cite{Kamihara} it has a striking novel feature that approximately two different energy gaps open on different pieces of the Fermi surface. Accompanied with theoretical predictions\cite{Brandt03,Brandt04} this multi-gap structure has been established within a short period by specific heat experiments\cite{Wang01,Butera01}, point-contact spectroscopy\cite{Brinkman01,Brinkman02}, and scanning tunneling microscope\cite{Kubler01,Kubler02,samuely01}. The larger gap opens on cylindrical Fermi surfaces of the $\sigma$-band with $2\Delta_{\sigma}(0)/k_BT_c = 3.6 - 4.5$, whereas the smaller one has the size $2\Delta_{\pi}(0)/k_BT_c = 1.1 - 1.5$ on three dimensional Fermi surfaces of the $\pi$-band.

Impurity effects of this material are very interesting to study. According to Anderson’s theorem for classic $s$-wave superconductors\cite{Anderson61,Anderson62}, nonmagnetic impurities do not affect superconducting properties in zero magnetic field. However, it was shown later by Markowitz and Kadanoff\cite{Markowitz62} that $T_c$ is actually reduced in the presence of gap anisotropy and impurity scattering. An application to a two-band model is due to Golubov and Mazin\cite{Golubov99}. Indeed, they predicted a rather drastic decrease of $T_c$ due to the interband impurity scattering. They also found that, as the interband scattering increases, the density of states changes from the two-gap structure inherent to the two-band model to the conventional single-gap structure. This reduction of $T_c$ has been confirmed recently by a couple of experiments. Wang et al.\cite{Wang01} measured the specific heat of polycrystalline MgB$_2$ after irradiation. They found both suppression of $T_c$ and a tendency towards a single-gap structure as the scattering is increased by irradiation. Lee et al.\cite{Lee01} clarified the possibility of complete suppression of superconductivity by replacing B in MgB$_2$ by C. However, few quantitative calculations have been performed on the impurity effects based on a realistic model for MgB$_2$\cite{Choi01}. For example, the specific heat has been calculated by Choi et al.\cite{Choi01} and Golubov et al.\cite{Golubov99} based on the clean-limit Eliashberg equation to obtain excellent quantitative agreements. However, no detail study has been performed for the specific heat from clean to dirty limits based on a microscopic model.

With these observation, we investigate nonmagnetic impurity effects in MgB$_2$. We thereby clarify impurity-concentration dependence of the quasiparticle density of states and the specific heat, choosing the parameters in the model suitable for MgB$_2$. Section II gives the formulation. Section III presents calculated results. Section IV summarizes the paper. We put $\hbar = k_B = 1$ throughout.

II. FORMULATION

A. Quasiclassical equations

We start from the Eilenberger equations\cite{Eilenberger60} for the Suhl-Matthias-Walker model\cite{Suhl60} with impurities, which form one of the most convenient frameworks to study impurity effects of the two-band model. We here adopt the formulation on the real energy axis instead of using Matsubara frequencies, which has an advantage that the free-energy functional can be defined unambiguously.

The Eilenberger equation on the real energy axis is given for the uniform case by

$$
\left(-i\epsilon + \sum_{\beta} \left( \frac{g_{\alpha\beta}^R}{2\tau_{\alpha\beta}} \right) \right) f_{\alpha}^R = \left( \Delta_{\alpha} + \sum_{\beta} \frac{f_{\alpha\beta}^R}{2\tau_{\alpha\beta}} \right) g_{\alpha}^R. \tag{1}
$$

Here $f_{\alpha}^R \equiv f_{\alpha}^R(\epsilon, \mathbf{k}_F)$ and $g_{\alpha}^R \equiv g_{\alpha}^R(\epsilon, \mathbf{k}_F)$ are retarded quasiclassical Green’s functions specified by the band index $\alpha (= \sigma, \pi)$ and the Fermi wave vector $\mathbf{k}_F$. They are connected by $g_{\alpha}^R = (1 - f_{\alpha}^R f_{\alpha}^R)^{1/2}$ with $f_{\alpha}^R(\epsilon, \mathbf{k}_F) = f_{\alpha}^R(-\epsilon, -\mathbf{k}_F)$. The symbol $\langle \cdot \rangle$ denotes the average over the Fermi surface for the relevant band with $\langle 1 \rangle = 1$. The quantity $\tau_{\alpha\beta}$ is the relaxation time for the nonmagnetic impurity scattering from $\alpha$- to $\beta$-band; they satisfy $\frac{1}{\tau_{\alpha\beta}} = \frac{N_s(0)}{N_\alpha(0)} \frac{1}{\tau_{\alpha}}$, where $N_s(0)$ is the normal-state density of states at the Fermi energy for the $\alpha$-band. Finally, $\Delta_{\alpha}$
is determined self-consistently by
\[ \Delta_\alpha = \sum_\beta \frac{\lambda_{\alpha\beta}}{2i} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \langle f_{\beta}^R(\varepsilon, k_F) \rangle, \]  
(2)
where \( \varepsilon_c \) is the cutoff energy, \( \phi(\varepsilon) \equiv \tanh(\varepsilon/2T) \), and \( \lambda_{\alpha\beta} \) is dimensionless coupling constant with \( \lambda_{\alpha\beta} = \frac{N_\alpha(0)}{N_\alpha(T)} \lambda_{\alpha\beta} \).

The functional for the free-energy difference corresponding to Eqs. (1) and (2) are given by
\[
F_s - F_n = \sum_{\alpha(\neq \beta)} N_\alpha(0) \left\{ \frac{|\Delta_\alpha|^2}{\lambda_{\alpha\alpha}} - \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \langle I_\alpha(\varepsilon) \rangle \right. \\
\left. - \frac{\lambda_{\alpha\beta}}{\lambda_{\alpha\alpha}^2} \frac{1}{2i} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \left[ \Delta_\alpha^* \langle f_{\beta}^R(\varepsilon) \rangle + \Delta_\alpha \langle f_{\beta}^R(\varepsilon) \rangle \right] \right. \\
\left. \times \frac{1}{(2\pi)^2} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon d\varepsilon' \phi(\varepsilon)\phi(\varepsilon') \right. \\
\left. \times \frac{\left[ \lambda_{\alpha\beta}^2 \langle f_{\beta}^R(\varepsilon) \rangle \langle f_{\beta}^R(\varepsilon') \rangle + \lambda_{\alpha\beta}^2 \langle f_{\beta}^R(\varepsilon) \rangle \langle f_{\beta}^R(\varepsilon') \rangle \right]}{2\tau_{\alpha\beta}} \\
\left. \right. \right\},
\]  
(3)
with
\[
\langle f_{\beta}^R(\varepsilon) \rangle = \frac{\sum_{s} N_\alpha(0) \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \langle I_\alpha(\varepsilon) \rangle \rangle}{N_\alpha(0) \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \langle I_\alpha(\varepsilon) \rangle}.
\]  
(4)

Equation (3) is a direct extension of Eilenberger’s free-energy functional to the two-band model. Indeed, variations of \( F_s - F_n \) with respect to \( f_{\alpha}^R \) and \( \Delta_\alpha^* \) lead to Eqs. (1) and (2), respectively.

The entropy is obtained from this free-energy functional by \( S_s = S_n - \partial(F_s - F_n)/\partial T \). Noting the stationarity of \( F_s - F_n \) with respect to \( f_{\alpha}^R \) and \( \Delta_\alpha^* \), we only have to differentiate with respect to the explicit temperature dependence in \( \phi(\varepsilon) = \tanh(\varepsilon/2T) \). We thereby obtain an explicit analytic expression for the entropy as
\[
S_s = S_n + \sum_{\alpha(\neq \beta)} N_\alpha(0) \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \frac{\partial \phi(\varepsilon)}{\partial T} \left\{ \langle I_\alpha(\varepsilon) \rangle \right. \\
\left. + \langle f_{\beta}^R(\varepsilon) \rangle \langle f_{\beta}^R(\varepsilon) \rangle + \langle g_{\alpha}^R(\varepsilon) \rangle \langle g_{\beta}^R(\varepsilon) \rangle - 1 \right\} \frac{1}{2\tau_{\alpha\beta}}.
\]  
(5)

In deriving this expression, we have used Eq. (2). Finally, the specific heat is calculated by numerically differentiating Eq. (3) as
\[
C_s = C_n + T \frac{d(S_s - S_n)}{dT}.
\]  
(6)

Equations (5) and (6) form a convenient and efficient starting point to calculate the specific heat for various impurity concentrations.

There is a disadvantage in the coupled self-consistency equations (1) and (2) that they may not be very stable numerically. However, it can be removed when \( \varepsilon_c \) is much larger than both \( \Delta_\alpha \) and \( 1/\tau_{\alpha\beta} \). This condition is well satisfied in MgB_2 where \( \varepsilon_c \) corresponds to the Deybe energy \( \omega_D \sim 1000 K \). Then using the asymptotic property \( f_{\alpha}^R \to \Delta_\alpha/(-i\varepsilon) \) as \( |\varepsilon| \to \infty \), Eq. (2) is transformed as
\[
\Delta_\alpha = \sum_\beta \frac{\lambda_{\alpha\beta}}{2i} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \langle \langle f_{\beta}^R(\varepsilon, k_F) \rangle - \frac{\Delta_\beta}{i\varepsilon} \rangle \\
+ \sum_\beta \frac{\lambda_{\alpha\beta}}{2} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) \langle \Delta_\beta \rangle \\
= 2\pi T \sum_\beta \lambda_{\alpha\beta} \sum_{n=0}^{\infty} \langle f_{\beta}(\varepsilon_n, k_F) \rangle - \frac{\Delta_\beta}{\varepsilon_n} \\
+ \sum_\beta \lambda_{\alpha\beta} \Delta_\beta \ln \left( \frac{2e^\gamma \varepsilon_c}{\pi T} \right),
\]  
(7)
where \( \gamma = 0.577 \) is the Euler constant, \( \varepsilon_n \equiv (2n+1)\pi T \) is the Matsubara frequency, and \( f_{\alpha}(\varepsilon_n) = f_{\alpha}^R(i\varepsilon_n) \). The limit \( \varepsilon_c \to \infty \) has been taken safely in the first integral to transform the integration into the summation over Matsubara frequencies. Equation (7) tells us that \( \Delta_\alpha \) has no angular dependence within the band. It then follows that \( f_{\alpha} \) neither has any angular dependence, so that \( \langle f_{\alpha} \rangle = f_{\alpha} \), and \( \langle g_{\alpha} \rangle = g_{\alpha} \). Hence Eq. (1) with \( \varepsilon \to i\varepsilon_n \) is simplified into
\[
\varepsilon_n + \frac{g_\beta}{2\tau_{\alpha\beta}} f_{\alpha} = \left( \Delta_\alpha + \frac{g_\beta}{2\tau_{\alpha\beta}} \right) g_{\alpha} \quad (\beta \neq \alpha).
\]  
(8)
Thus, the intraband scattering does not affect superconductivity in zero magnetic field at all, in agreement with Anderson’s theorem.\(^{26}\) Equation (3) could be presented at the beginning in place of Eq. (1). However, Eqs. (1) - (3) have an advantage that they could easily be extended to nonuniform systems by simply adding gradient terms.\(^{26,28}\)

Equations (7) and (8) enable us to obtain \( \Delta_\alpha \) from calculations on Matsubara frequencies, which are numerically more stable than Eqs. (1) and (2). Once \( \Delta_\alpha \) is fixed in this way, the density of states is calculated by solving Eq. (1) as
\[
N(\varepsilon) = \sum_\alpha N_\alpha(0) \text{Re} g_{\alpha}^R(\varepsilon).
\]  
(9)

### B. Transition temperature

We now derive the \( T_c \) equation valid at all impurity concentrations. To this end, we expand \( f_{\alpha} \) and \( g_{\alpha} \) up to first order in \( \Delta_\beta \) as \( f_{\alpha} = f_{\alpha}^{(1)} \) and \( g_{\alpha} = 1 \). Substituting

\[
C_s = C_n + T \frac{d(S_s - S_n)}{dT}.
\]  
(6)
them into Eq. (9), we obtain $f^{(1)}_\alpha$ as

$$f^{(1)}_\alpha = \sum_\beta h_{\alpha\beta} \Delta_\beta,$$

where $h_{\alpha\beta}$ is defined by

$$h_{\alpha\beta} = \delta_{\alpha\beta} \left( \frac{n_\alpha}{\varepsilon_n} + \frac{1-n_\alpha}{\varepsilon_n + 1} \right) + (1-\delta_{\alpha\beta}) \left( \frac{n_\beta}{\varepsilon_n} - \frac{n_\beta}{\varepsilon_n + 1} \right),$$

(11)

with

$$n_\alpha = \frac{N_\alpha(0)}{N_\alpha(0) + N_\beta(0)}, \quad \frac{1}{\tau} = \frac{1}{2\tau_{\alpha\beta}} + \frac{1}{2\tau_{\beta\alpha}}.$$  

(12)

Substituting Eq. (11) into Eq. (7), we obtain the condition for a nontrivial solution as

$$\det(\mathbf{1} - \mathbf{H}) = 0,$$

(13)

where the matrix $\mathbf{H}$ is defined by

$$H_{\alpha\beta} = \sum_\gamma \lambda_\gamma \left\{ 2\pi T_c \frac{n_\alpha}{\varepsilon_n} \ln \left[ \frac{\Gamma(2\varepsilon_n) - \delta_{\gamma\beta}}{\varepsilon_n} \right] + \delta_{\gamma\beta} \ln \left( \frac{2\varepsilon_n}{\pi T_c} \right) \right\}.$$  

(14)

By solving Eq. (13), $T_c$ is obtained for an arbitrary $\tau$. Notice that all the summations in Eq. (13) can be expressed in terms of the digamma function $\psi(x)$.

When $T_c \tau \ll 1$, Eq. (13) can be solved explicitly by using the asymptotic expression $\psi(x) \sim \ln x (x \to \infty)$ as

$$T_c = \frac{2\varepsilon_c}{\pi} e_\pi \exp \left[ \sum_{\alpha(\neq \beta)} (\lambda_{\alpha\beta} n_\alpha - \lambda_{\alpha\alpha} n_\beta) \ln(\varepsilon_\alpha \tau) + 1 \right] \left[ (\lambda_{\alpha\alpha} \lambda_{\pi\pi} - \lambda_{\sigma\sigma} \lambda_{\pi\sigma}) \ln(\varepsilon_\pi \tau) - \sum_\alpha \lambda_\alpha n_\alpha \right],$$

(15)

with $\lambda_\alpha = \sum_\beta \lambda_{\alpha\beta}$. This expression is useful to see whether $T_c$ is suppressed completely or not as the interband scattering increases.

C. Density of states in the dirty limit

We now derive an analytic expression for the density of states in the dirty limit of $T_c \tau \ll 1$. In this case with $\varepsilon \ll T_c$, we can neglect the first terms on both sides of Eq. (7). It then follows that $f^R_\alpha/g^R_\alpha = f^R_\beta/g^R_\beta$, or equivalently, $f^R_\alpha = f^R_\beta \equiv f^R$ and $g^R_\alpha = g^R_\beta \equiv g^R$. The quantities $f^R$ and $g^R$ are obtained easily as

$$f^R(\varepsilon) = \frac{\Delta}{\sqrt{\Delta^2 - \varepsilon^2}}, \quad g^R(\varepsilon) = \frac{-i\varepsilon}{\sqrt{\Delta^2 - \varepsilon^2}},$$

(16)

where $\varepsilon_+ \equiv \varepsilon + i0_+$, and $\Delta$ is defined by

$$\Delta = n_\sigma \Delta_\sigma + n_\pi \Delta_\pi.$$  

(17)

### Table I: Coupling constants

| Case | $\lambda_{\sigma\sigma}$ | $\lambda_{\sigma\pi}$ | $\lambda_{\sigma\sigma}$ | $\lambda_{\pi\pi}$ |
|------|--------------------------|------------------------|--------------------------|---------------------|
| A    | $2.45 \times 10^{-4}$    | $5.95 \times 10^{-4}$  | $4.28 \times 10^{-4}$   | $1.10 \times 10^{-4}$ |
| B    | $2.25 \times 10^{-4}$    | $2.35 \times 10^{-4}$  | $1.69 \times 10^{-4}$   | $1.22 \times 10^{-4}$ |

It hence follows that the density of states $\propto \text{Re} \gamma^R$ has the conventional BCS structure, diverging at $\varepsilon = \pm \Delta$. The corresponding pair potential is determined by

$$\Delta_\alpha = \frac{\lambda_\alpha}{2i} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \phi(\varepsilon) f^R(\varepsilon),$$

(18)

as already pointed out by Golubov and Mazin. Thus, the ratio of the two pair potentials is given by $\Delta_\sigma/\Delta_\pi = \lambda_\sigma/\lambda_\pi$.

D. Numerical procedures

There are five parameters in the model:

$$\lambda_{\sigma\sigma}, \quad \lambda_{\sigma\pi}, \quad \lambda_{\pi\pi}, \quad \varepsilon_c, \quad N_\sigma(0)/N_\pi(0).$$  

(19)

They are fixed so as to reproduce experiments on MgB$_2$ as closely as possible. To be more specific, the ratio $N_\sigma(0)/N_\pi(0)$ is set equal to 0.72 following an electronic-structure calculation. As for the coupling constants, we use Eq. (2) in the clean limit at $T = 0, T_c$ which yields

$$1 = \lambda_{\sigma\sigma} \ln \left( \frac{2\varepsilon_c}{\Delta_{\sigma}} \right) + \lambda_{\sigma\pi} \frac{\Delta_{\sigma}}{\Delta_{\sigma}} \ln \left( \frac{2\varepsilon_c}{\Delta_{\sigma}} \right) - \ln \left( \frac{\Delta_{\sigma}}{\Delta_{\sigma}} \right),$$

(20a)

$$\frac{\Delta_{\sigma}}{\Delta_{\sigma}} = \lambda_{\sigma\pi} \ln \left( \frac{2\varepsilon_c}{\Delta_{\sigma}} \right) + \lambda_{\pi\pi} \frac{\Delta_{\sigma}}{\Delta_{\sigma}} \ln \left( \frac{2\varepsilon_c}{\Delta_{\sigma}} \right) - \ln \left( \frac{\Delta_{\sigma}}{\Delta_{\sigma}} \right),$$

(20b)

and

$$\ln \left( \frac{2\varepsilon_c}{\pi T_c} \right) = \frac{\lambda_{\sigma\sigma} + \lambda_{\sigma\pi} + \sqrt{\lambda_{\sigma\sigma} - \lambda_{\sigma\pi}}^2 + 4 \lambda_{\sigma\pi} \lambda_{\pi\pi}}{2(\lambda_{\sigma\sigma} \lambda_{\pi\pi} - \lambda_{\sigma\pi} \lambda_{\pi\pi})},$$

(20c)

respectively. These equations are used to eliminate $\lambda_{\alpha\beta}$ in favor of $\Delta_{\sigma\sigma}/\Delta_{\sigma\sigma}, T_c/\Delta_{\sigma\sigma},$ and $\varepsilon_c/\Delta_{\sigma\sigma}$, where $\Delta_{\sigma\sigma}, \Delta_{\sigma\sigma}$ denotes $\Delta_{\sigma\sigma}, \Delta_{\sigma\sigma}$ in the clean limit.

We here consider the following two cases:

Case A: $T_c/\Delta_{\sigma\sigma} = 0.50; \Delta_{\sigma\sigma}/\Delta_{\pi\pi} = 3.00; \varepsilon_c/\Delta_{\sigma\sigma} = 20.0,$

(21a)

Case B: $T_c/\Delta_{\sigma\sigma} = 0.48; \Delta_{\sigma\sigma}/\Delta_{\pi\pi} = 2.95; \varepsilon_c/\Delta_{\sigma\sigma} = 10.0.$

(21b)

These values are chosen so as to reproduce temperature dependence of the observed energy gaps on clean
samples$^{14,15,16,18}$ as closely as possible. The corresponding coupling constants are listed in Table I. It has been found that the whole results are rather insensitive to $\varepsilon_c$, as may be expected.

Numerical calculations have been performed as follows. First, $f_\alpha$ and $g_\alpha$ with $f_\alpha^2 + g_\alpha^2 = 1$ are expressed conveniently in terms of a single function $a_\alpha$ as

$$f_\alpha = \frac{2a_\alpha}{1 + a_\alpha^2}, \quad g_\alpha = \frac{1 - a_\alpha^2}{1 + a_\alpha^2}.$$  \hfill (22)

Substituting Eq. (22) and a trial $(\Delta_\sigma, \Delta_\pi)$ into it, Eq. (8) is transformed into a set of nonlinear equations for $a_\alpha$, which may be solved by using one of the standard numerical procedures.$^{21}$ The obtained $f_\alpha$ is then substituted into Eq. (11) to find a new $(\Delta_\sigma, \Delta_\pi)$. This procedure is repeated until the convergence is reached. The pair potentials thereby obtained are then used in Eq. (11) to calculate $f^R$ and $g^R$ on the real energy axis. Finally, those $f^R$ and $g^R$ are substituted into Eqs. (5), (6), and (9) to calculate the specific heat and the density of states.

III. RESULTS

Figure 1 plots $T_c$ as a function of the interband scattering specified by $\log_{10}(\Delta_{\sigma0}\tau_{\sigma\pi})$ for the two cases of Eq. (21). Here $T_c$ is normalized by $T_{c0}$ without the interband
scattering. We observe that $T_c$ drops steeply around $\tau_{\pi\pi} = \Delta_0^{-1}$ in both cases. However, whereas $T_c$ in Case A remains finite for $\tau_{\pi\pi} \to 0$, $T_c$ in Case B decreases to zero at a finite $\tau_{\pi\pi}$. This difference can be realized from Eq. (15) where the term in the square bracket passes through negative infinity for $T_c \to 0$. It is interesting to see experimentally whether $T_c$ of MgB$_2$ is suppressed completely or not by increasing the interband scattering, although this may not be easy.

Figure 4 shows temperature dependence of the pair potentials for (a) Case A and (b) Case B. In both cases, the pair potentials decrease as $\tau_{\pi\pi}$ becomes shorter. However, the two pair potentials do not approach to a single value even for $\tau_{\pi\pi} \to 0$. Notice also that the pair potentials are not directly connected with any observable quantities except in the clean limit.

Figure 5 shows the density of states at $T/T_c = 0.01$ for (a) Case A and (b) Case B. In the clean limit $\Delta_0 \tau_{\pi\pi} = 10000.0$, we clearly observe a couple of divergences at $\varepsilon = \Delta_\sigma$, $\Delta_\pi$. As the interband scattering becomes larger, the divergences are smeared to finite peaks, which eventually merge into a single peak in the dirty limit at $\varepsilon = \Delta$ given by Eq. (17). Notice that the excitation threshold is not a monotonic function of $\tau_{\pi\pi}$; for Case A, for example, the threshold is seen to increase as $\tau_{\pi\pi}$ becomes smaller.

Figure 4 plots the specific heat as a function of $T/T_c$ in (a) Case A and (b) Case B for $\Delta_0 \tau_{\pi\pi} = 10000.0$, 1.0, 0.1. A shoulder is clearly seen around $T/T_c = 0.2$ for $\Delta_0 \tau_{\pi\pi} = 10000.0$, corresponding to the divergence at $\varepsilon = \Delta_\pi$ in Fig. 6. It gradually disappears as $\tau_{\pi\pi}$ becomes shorter, however, and we finally have a conventional single-exponential behavior in the dirty limit.

Finally, Fig. 5 compares the present theory with the specific-heat experiment after irradiation performed by Wang et al. The data points correspond to measurements before irradiation (top), after the first irradiation (middle), and after the second irradiation (bottom), where the former two are shifted upwards by 1.5$C_n$ and 0.75$C_n$, respectively. The curves of Fig. 5(a) are obtained by using the parameters of Case A with $\Delta_0 \tau_{\pi\pi} = 50.0, 7.0, 4.0$ from top to bottom, respectively. On the other hand, those of Fig. 5(b) correspond to Case B with $\Delta_0 \tau_{\pi\pi} = 10000.0, 30.0, 1.0$. The agreements are good.
for both cases, especially for Case B. From these comparisons, we realize that the interband scattering after the second irradiation is still not very strong with $\Delta_{0}/\tau_{\sigma\pi} \gtrsim 1.0$. The fact may imply the difficulty of introducing the interband impurity scattering in MgB$_2$. This tendency is also seen in the carbon-substituted system Mg(B$_{2-x}$C$_x$)$_2$ where the two-gap structure is still observed clearly for $x \sim 0.1$. Thus, the large reduction of $T_c$ observed in Mg(B$_{2-x}$C$_x$)$_2$ by Lee et al should be attributed not only to the interband scattering alone but also to a change of the pairing interaction due to the electronic structure.

IV. CONCLUSION

We have studied nonmagnetic impurity effects for MgB$_2$ based on the quasiclassical equations of superconductivity for the Suhl-Matthias-Walker model. The parameters in the model are fixed so as to reproduce experimental values for $\Delta_{0}/\Delta_{0}$ and $\Delta_{0}/T_c$. The interband impurity scattering tends to reduce the gap anisotropy. We have clarified how the density of states changes from the two-gap structure in the clean limit to the single-gap structure in the dirty limit with strong interband scattering. Especially, there may be cases where the excitation threshold increases as the scattering becomes stronger. Calculated curves for the specific heat agree well with measurements before and after irradiation. This comparison has also enabled us to estimate the relaxation time $\tau_{\sigma\pi}$ for the interband scattering. It satisfies $\tau_{\sigma\pi} \gtrsim 1/\Delta_{0}$ even after the second irradiation, implying the difficulty of introducing the interband scattering in this system.

Acknowledgments

This work is supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science, and Technology of Japan.
33 A. Shibata, M. Matsumoto, K. Izawa, and Y. Matsuda, private communications.