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Entropy and spin susceptibility of *s*-wave type-II superconductors near H_{c2}

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A theoretical study is performed on the entropy S_s and the spin susceptibility χ_s near the upper critical field H_{c2} for *s*-wave type-II superconductors with arbitrary impurity concentrations. The changes of these quantities through H_{c2} may be expressed as $[S_s(T,B)-S_s(T,0)]/[S_n(T)-S_s(T,0)]=1-\alpha_S(1-B/H_{c2})\approx(B/H_{c2})^{\alpha_S}$, for example, where B is the average flux density and S_n denotes entropy in the normal state. It is found that the slopes α_S and α_χ at $T=0$ are identical, connected directly with the zero-energy density of states, and vary from 1.72 in the dirty limit to 0.5–0.6 in the clean limit. This mean-free-path dependence of α_S and α_χ at $T=0$ is quantitatively the same as that of the slope $\alpha_\rho(T=0)$ for the flux-flow resistivity studied previously. The result suggests that $S_s(B)$ and $\chi_s(B)$ near $T=0$ are convex downward (upward) in the dirty (clean) limit, deviating substantially from the linear behavior $\propto B/H_{c2}$. The specific-heat jump at H_{c2} also shows fairly large mean-free-path dependence.

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I. INTRODUCTION

This paper considers the changes of the entropy S_s and the spin susceptibility χ_s through H_{c2} for classic *s*-wave type-II superconductors. These quantities were calculated by Maki[1,2] in the dirty limit for superconducting alloys nearly 40 years ago. However, detailed studies on clean systems are still missing even for *s*-wave superconductors. Writing these quantities as

$$\frac{S_s(T,B)-S_s(T,0)}{S_n(T)-S_s(T,0)}=1-\alpha_S\left(1-\frac{B}{H_{c2}}\right)\approx\left(\frac{B}{H_{c2}}\right)^{\alpha_S}, \quad (1a)$$

$$\frac{\chi_s(T,B)-\chi_s(T,0)}{\chi_n(T)-\chi_s(T,0)}=1-\alpha_\chi\left(1-\frac{B}{H_{c2}}\right)\approx\left(\frac{B}{H_{c2}}\right)^{\alpha_\chi}, \quad (1b)$$

the slopes α_S and α_χ will be obtained quantitatively for arbitrary impurity concentrations. The results near H_{c2} will also be useful for getting an insight into the behaviors over $0\leqslant B\leqslant H_{c2}$. Indeed, $\alpha>1$ ($\alpha<1$) indicates overall field dependence which is convex downward (upward), as seen from Eq. (1).

It seems to have been widely accepted that various physical quantities of classic *s*-wave type-II superconductors follow the linear field dependence with $\alpha=1$ at low temperatures. A theoretical basis for it is the density of states for a single vortex calculated by Caroli, de Gennes, and Matricon.[3,4] However, few quantitative calculations have been carried out so far on the explicit field dependence. Recently, Ichioka *et al.*[5] performed a numerical study on the density of states of clean two-dimensional *s*-wave superconductors with $\kappa\gg1$ at $T=0.5T_c$. They found the exponent $\alpha=0.67$ for the overall field dependence of the zero-energy density of states. Also, experiments on the *T*-linear specific-heat coefficient $\gamma_s(B)$ for clean V_3Si,[6] $NbSe_2$,[7–10] and $CeRu_2$[11] show marked upward deviations from the linear behavior $\gamma_n B/H_{c2}$. Even early experiments on $\gamma_s(B)$ for clean V and Nb indicate similar deviations,[12,13] although not recognized explicitly in those days due to the absence of a theory on clean systems. These results indicate that the field dependence with $\alpha<1$ is a general feature of clean *s*-wave superconductors, as suggested by Ramirez.[6]

Following the preceding works on the Maki parameters[14] and the flux-flow resistivity,[15] which will be referred to as I and II, respectively, I here present a detailed study on S_s and χ_s near H_{c2} at all temperatures. I thereby hope to clarify the κ and mean-free-path (l_{tr}) dependence of α_S and α_χ. Calculations are performed for both two- and three-dimensional isotropic systems to see the dependence of α_S and α_χ on detailed Fermi-surface structures. I also calculate the specific-heat jump at H_{c2} for various values of κ and l_{tr}. To my knowledge, this kind of a systematic study has not been performed even for classic *s*-wave superconductors.

Unlike the convention, I adopt the average flux density B in the bulk as an independent variable instead of the external field H. An advantage for it is that the irrelevant region $H\leqslant H_{c1}$ is automatically removed from the discussion on the field dependence. This distinction between B and H becomes important for low-κ materials where $H\leqslant H_{c1}$ occupies a substantial part of $0\leqslant H\leqslant H_{c2}$. Any experiment on the B dependence should be accompanied by a careful measurement on the magnetization, especially for low-κ materials such as Nb and V.

Section II provides the formulation, Sec. III presents numerical results, and Sec. IV summarizes the paper. The main analytic results are tabulated in Table I for an easy reference. I put $k_B=1$ throughout.

II. FORMULATION

A. Entropy and Pauli paramagnetism

As before,[14,15] I consider the *s*-wave pairing with an isotropic Fermi surface and *s*-wave impurity scattering in an external magnetic field $\mathbf{H}\|\mathbf{z}$. The formulation proceeds in exactly the same way for both the three-dimensional system and the two-dimensional system placed in the xy plane perpendicular to $\mathbf{H}$. The vector potential in the bulk can be written as[16–21]

$$\mathbf{A}(\mathbf{r})=Bx\hat{\mathbf{y}}+\tilde{\mathbf{A}}(\mathbf{r}), \quad (2)$$

TABLE I. Main analytic results for the entropy $S_{\rm s}$, the spin susceptibility $\chi_{\rm s}$, dH_{c2}/dT, and the specific-heat jump ΔC at H_{c2}, together with relevant quantities.

	$0\leq B\leq H_{c2}$	$B\lesssim H_{c2}$	$B\lesssim H_{c2}$, $T\to 0$	$B\lesssim H_{c2}$, $T\to 0$, $\tau\to 0$
$S_{\rm s}$	Eq. (7)	Eq. (14a) or (19)	Eq. (26a)	Eq. (37a)
$\chi_{\rm s}$	Eq. (10)	Eq. (14b)	Eq. (26b)	Eq. (37b)
dH_{c2}/dT		Eq. (20)		Eq. (34)
ΔC		Eq. (21)		
Δ_0		Eq. (13a)		Eq. (36)
$\tilde f_N^{(1)}$		Eqs. (13b) and (22)		Eq. (30)
$\partial\tilde f_N^{(1)}/\partial H_{c2}$		Eq. (17)		
$\partial\tilde f_N^{(1)}/\partial\varepsilon_n$		Eq. (18)		

where B is the average flux density produced jointly by the external current and the supercurrent inside the sample, and $\tilde{\mathbf{A}}$ expresses the spatially varying part of the magnetic field satisfying $\int\boldsymbol{\nabla}\times\tilde{\mathbf{A}}\,d\mathbf{r}=\mathbf{0}$.

I first write down the expressions for the entropy and the magnetization in the presence of Pauli paramagnetism. This effect can be included in the Eilenberger equations[22] for the quasiclassical Green's functions f, $f^\dagger$, and g by the replacement[23–25]

$$\varepsilon_n\to\varepsilon_n'\equiv\varepsilon_n-i\mu_{\rm B}\hat{\mathbf{z}}\cdot(\boldsymbol{\nabla}\times\mathbf{A}),\tag{3}$$

where $\varepsilon_n\equiv(2n+1)\pi T$ is the Matsubara energy and $\mu_{\rm B}$ is the Bohr magneton. Choosing B as an independent variable and measuring the energy from the normal state at the same temperature T in zero field, the corresponding Eilenberger's free-energy functional[22] is given by

$$F=\int d\mathbf{r}\left\{\frac{(\boldsymbol{\nabla}\times\mathbf{A})^2}{8\pi}-\frac{\chi_{\rm n}}{2}(\boldsymbol{\nabla}\times\mathbf{A})^2+N(0)|\Delta(\mathbf{r})|^2\ln\frac{T}{T_c}+\pi TN(0)\sum_{n=-\infty}^{\infty}\left[\frac{|\Delta(\mathbf{r})|^2}{|\varepsilon_n|}-\langle I(\varepsilon_n,\mathbf{k}_{\rm F},\mathbf{r})\rangle\right]\right\}.\tag{4}$$

Here $\chi_{\rm n}=2\mu_{\rm B}^2N(0)$ is the normal-state spin susceptibility with $N(0)$ the density of states per one spin and per unit volume at the Fermi level, Δ is the pair potential, $\mathbf{k}_{\rm F}$ is the Fermi wave vector, and $\langle\cdots\rangle$ denotes the Fermi-surface average with $\langle 1\rangle=1$. The quantity I is defined by[14]

$$I\equiv\Delta^*f+\Delta f^\dagger+2\varepsilon_n'[g-\mathrm{sgn}(\varepsilon_n)]+\hbar\frac{f\langle f^\dagger\rangle+\langle f\rangle f^\dagger}{4\tau}+\hbar\frac{g\langle g\rangle-1}{2\tau}-\hbar\frac{f^\dagger\mathbf{v}_{\rm F}\cdot\boldsymbol{\partial}f-f\mathbf{v}_{\rm F}\cdot\boldsymbol{\partial}^*f^\dagger}{2[g+\mathrm{sgn}(\varepsilon_n)]},\tag{5}$$

where τ is the relaxation time in the second-Born approximation, $\mathbf{v}_{\rm F}$ is the Fermi velocity, and $\boldsymbol{\partial}$ denotes

$$\boldsymbol{\partial}\equiv\boldsymbol{\nabla}-i\frac{2e}{\hbar c}\mathbf{A}.\tag{6}$$

The quasiclassical Green's functions f and g are connected by $g=(1-ff^\dagger)^{1/2}\,\mathrm{sgn}(\varepsilon_n)$ with $f^\dagger(\varepsilon_n,\mathbf{k}_{\rm F},\mathbf{r})=f^*(-\varepsilon_n,\mathbf{k}_{\rm F},\mathbf{r})$. The functional derivatives of Eq. (4) with respect to $f^\dagger$, Δ^*, and $\tilde{\mathbf{A}}$ lead to the Eilenberger equation for f, the self-consistency equation for $\Delta(\mathbf{r})$, and the Maxwell equation for $\tilde{\mathbf{A}}$, respectively.

The expression of the entropy $S_{\rm s}$ is obtained from Eq. (4) by the thermodynamic relation. $S_{\rm s}=S_{\rm n}-\partial F/\partial T$. Considering the stationarity with respect to f, Δ, and $\tilde{\mathbf{A}}$, we only have to differentiate F with respect to the explicit temperature dependence. We thereby obtain

$$S_{\rm s}=S_{\rm n}-\frac{N(0)}{T}\int d\mathbf{r}\left[|\Delta(\mathbf{r})|^2-\pi T\sum_{n=-\infty}^{\infty}\langle I(\varepsilon_n,\mathbf{k}_{\rm F},\mathbf{r})\rangle-2\pi T\sum_{n=-\infty}^{\infty}\varepsilon_n\langle g-\mathrm{sgn}(\varepsilon_n)\rangle\right],\tag{7}$$

where $S_{\rm n}=2\pi^2N(0)VT/3$ with V the volume of the system. In contrast, the expression of the external field H may be derived by applying the Doria-Gubernatis-Rainer scaling to Eq. (4).[26] The details are given in Appendix A of I, and we obtain

$$H=-4\pi M_{\rm nP}+B+\frac{1}{BV}\int d\mathbf{r}(\boldsymbol{\nabla}\times\tilde{\mathbf{A}})^2+\frac{\pi^2TN(0)}{BV}\sum_{n=-\infty}^{\infty}\int d\mathbf{r}\left\langle\hbar\frac{f^\dagger\mathbf{v}_{\rm F}\cdot\boldsymbol{\partial}f-f\mathbf{v}_{\rm F}\cdot\boldsymbol{\partial}^*f^\dagger}{g+\mathrm{sgn}(\varepsilon_n)}\right\rangle+i\frac{8\pi^2TN(0)\mu_{\rm B}}{BV}\sum_{n=-\infty}^{\infty}\int d\mathbf{r}\langle g\rangle\hat{\mathbf{z}}\cdot(\boldsymbol{\nabla}\times\mathbf{A}),\tag{8}$$

where $M_{\rm nP}\equiv\chi_{\rm n}B$ denotes the normal-state magnetization due to Pauli paramagnetism. We thus arrive at the expression of the magnetization from Pauli paramagnetism as

$$M_{\rm sP}=M_{\rm nP}-i\frac{2\pi TN(0)\mu_{\rm B}}{BV}\sum_{n=-\infty}^{\infty}\int d\mathbf{r}\langle g\rangle\hat{\mathbf{z}}\cdot(\boldsymbol{\nabla}\times\mathbf{A}).\tag{9}$$

When Pauli paramagnetism is negligible compared with the orbital diamagnetism by supercurrent, we can take the limit $\mu_B\to 0$ in Eqs. (7) and (9) and retain only the leading-order terms. This procedure yields $\varepsilon_n'\to\varepsilon_n$ for Eq. (7). On the other hand, Eq. (9) is transformed by noting Eq. (3) into

$$M_{\rm sP}=M_{\rm nP}\left[1-\frac{\pi T}{V}\sum_{n=-\infty}^{\infty}\int d\mathbf{r}\frac{\partial\langle g\rangle}{\partial\varepsilon_n}\left(\frac{\boldsymbol{\nabla}\times\mathbf{A}}{B}\right)^2\right]. \quad (10)$$

If the zero-field expression $g=\varepsilon_n/\sqrt{\varepsilon_n^2+|\Delta|^2}$ is substituted into Eq. (10) with $\boldsymbol{\nabla}\times\mathbf{A}=B\hat{\mathbf{z}}$, the terms in the square bracket reduce to the Yosida function.[27]

B. Expressions near H_{c2}

I now consider the cases where Pauli paramagnetism is small and provide explicit expressions to Eqs. (7) and (10) near H_{c2}. From now on I adopt the units used previously[14,15] where the energy, the length, and the magnetic field are measured by the zero-temperature energy gap $\Delta(0)$ at $H=0$, the coherence length $\xi_0\equiv\hbar v_{\rm F}/\Delta(0)$ with $v_{\rm F}$ the Fermi velocity, and $B_0\equiv\phi_0/2\pi\xi_0^2$ with $\phi_0\equiv hc/2e$ the flux quantum, respectively, with $\hbar=1$.

First, f, g, and $\tilde{\mathbf{A}}$ are expanded up to the second order in $\Delta(\mathbf{r})$ as

$$f=f^{(1)},$$

$$g=(1-\tfrac{1}{2}f^{(1)\dagger}f^{(1)})\,{\rm sgn}(\varepsilon_n),$$

$$\tilde{\mathbf{A}}=\tilde{\mathbf{A}}^{(2)}. \quad (11)$$

Substituting them into Eqs. (7) and (10) and using the Eilenberger equations for $f^{(1)}$ and $f^{(1)\dagger}$ to remove terms with $\mathbf{v}_{\rm F}\cdot\boldsymbol{\partial}$, we obtain

$$\frac{S_{\rm s}}{S_{\rm n}}=1-\frac{3}{2\pi^2T^2V}\int d\mathbf{r}\left[|\Delta(\mathbf{r})|^2-\frac{\pi T}{2}\sum_n\langle f^{(1)\dagger}\Delta+f^{(1)}\Delta^*\rangle+\pi T\sum_n|\varepsilon_n|\langle f^{(1)\dagger}f^{(1)}\rangle\right], \quad (12a)$$

$$\frac{M_{\rm sP}}{M_{\rm nP}}=1+\frac{\pi T}{2V}\sum_n\int d\mathbf{r}\left\langle\frac{\partial f^{(1)\dagger}}{\partial\varepsilon_n}f^{(1)}+f^{(1)\dagger}\frac{\partial f^{(1)}}{\partial\varepsilon_n}\right\rangle{\rm sgn}(\varepsilon_n). \quad (12b)$$

Further, $\Delta(\mathbf{r})$ and $f^{(1)}$ near H_{c2} can be expanded in the basis functions $\psi_{N\mathbf{q}}(\mathbf{r})$ of the vortex lattice as[14]

$$\Delta(\mathbf{r})=\sqrt{V}\Delta_0\psi_{0\mathbf{q}}(\mathbf{r}), \quad (13a)$$

$$f^{(1)}(\varepsilon_n,\mathbf{k}_{\rm F},\mathbf{r})=\sqrt{V}\Delta_0\sum_{N=0}^{\infty}\tilde{f}_N^{(1)}(\varepsilon_n,\theta)\,e^{iN\varphi}\psi_{N\mathbf{q}}(\mathbf{r}), \quad (13b)$$

where (θ,φ) are the polar angles of $\mathbf{v}_{\rm F}$ with $\sin\theta\to1$ in two dimensions, N denotes the Landau level, and $\mathbf{q}$ is an arbitrary chosen magnetic Bloch vector characterizing the broken translational symmetry of the flux-line lattice and specifying the core locations.[21] The coefficients Δ_0 and $\tilde{f}_N^{(1)}$ are both real for the relevant hexagonal lattice. Substituting these expressions into Eqs. (12a) and (12b) and using the orthonormality of $\psi_{N\mathbf{q}}(\mathbf{r})$ and $e^{iN\varphi}$, we obtain

$$\frac{S_{\rm s}}{S_{\rm n}}=1-\frac{3\Delta_0^2}{2\pi^2T^2}\left[1-\pi T\sum_{n=-\infty}^{\infty}\langle\tilde{f}_0^{(1)}\rangle+\pi T\sum_{n=-\infty}^{\infty}|\varepsilon_n|\sum_N(-1)^N\langle\tilde{f}_N^{(1)}\tilde{f}_N^{(1)}\rangle\right], \quad (14a)$$

$$\frac{M_{\rm sP}}{M_{\rm nP}}=1+\pi T\Delta_0^2\sum_{n=-\infty}^{\infty}\sum_N(-1)^N\left\langle\frac{\partial\tilde{f}_N^{(1)}}{\partial\varepsilon_n}\tilde{f}_N^{(1)}\right\rangle{\rm sgn}(\varepsilon_n). \quad (14b)$$

Except $\Delta_0^2\propto H_{c2}-B$, all the quantities in Eqs. (14a) and (14b) are to be evaluated at H_{c2}.

It is possible to give an alternative convenient expression to Eq. (14a). To this end, we make use of the equation for H_{c2} obtained as Eq. (33) of I:

$$\ln\frac{T_c}{T}+\pi T\sum_{n=-\infty}^{\infty}\left[\langle\tilde{f}_0^{(1)}(\varepsilon_n)\rangle-\frac{1}{|\varepsilon_n|}\right]=0. \quad (15)$$

Differentiating Eq. (15) with respect to T yields

$$-1+\pi T\sum_n\left[\langle\tilde{f}_0^{(1)}\rangle+\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial\varepsilon_n}\varepsilon_n+\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial H_{c2}}T\frac{dH_{c2}}{dT}\right]=0. \quad (16)$$

The quantity $\partial\langle\tilde{f}_0^{(1)}\rangle/\partial H_{c2}$ has been calculated as Eqs. (31) and (32) of I:

$$\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial H_{c2}}=\sum_N(-1)^{N+1}\sqrt{\frac{N+1}{8H_{c2}}}\langle\tilde{f}_{N+1}^{(1)}\tilde{f}_N^{(1)}\sin\theta\rangle. \quad (17)$$

A similar procedure leads to the analytic expressions for $\partial\langle\tilde{f}_0^{(1)}\rangle/\partial\varepsilon_n$ and $\partial\tilde{f}_N^{(1)}/\partial\varepsilon_n$ in Eq. (14b) as

$$\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial\varepsilon_n}=-\sum_N(-1)^N\langle\tilde{f}_N^{(1)}\tilde{f}_N^{(1)}\rangle{\rm sgn}(\varepsilon_n), \quad (18a)$$

$$\frac{\partial\tilde{f}_N^{(1)}}{\partial\varepsilon_n}=-\sum_N K_N^{N'}\tilde{f}_{N'}^{(1)}+\frac{K_N^0}{2\tau}{\rm sgn}(\varepsilon_n)\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial\varepsilon_n}, \quad (18b)$$

where $K_N^{N'}$ is defined by Eq. (25) of I. Using Eqs. (16) and (18a) in Eq. (14a), we obtain

$$\frac{S_{\rm s}}{S_{\rm n}}=1-\frac{dH_{c2}}{dT}\frac{3\Delta_0^2}{2\pi}\sum_{n=-\infty}^{\infty}\frac{\partial\langle\tilde{f}_0^{(1)}(\varepsilon_n)\rangle}{\partial H_{c2}}, \quad (19)$$

with

$$\frac{dH_{c2}}{dT}=\frac{1-\pi T\sum_{n=-\infty}^{\infty}\left[\langle\tilde{f}_0^{(1)}\rangle+\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial\varepsilon_n}\varepsilon_n\right]}{\pi T^2\sum_{n=-\infty}^{\infty}\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial H_{c2}}}. \quad (20)$$

Equation (20) also enables us to calculate the specific-heat jump at H_{c2}. Indeed, it is given in conventional units as[1]

$$\Delta C = \frac{T}{4\pi}\left(\frac{dH_{c2}}{dT}\right)^2 \frac{1}{(2\kappa_2^2-1)\beta_{\rm A}}, \tag{21}$$

where κ_2 is the Maki parameter[14,28] and $\beta_{\rm A}=1.16$.

Equations (14) and (21) with Eqs. (17), (18), and (20) are the main analytic results of the paper. The quantities Δ_0, $\tilde{f}_N^{(1)}$, and κ_2 have been obtained in I. The explicit expression for $\tilde{f}_N^{(1)}$ is given by

$$\tilde{f}_N^{(1)} = \frac{\tilde{K}_N^0 \,{\rm sgn}(\varepsilon_n)}{1-\langle \tilde{K}_0^0\rangle {\rm sgn}(\varepsilon_n)/2\tau}, \tag{22}$$

where $\tilde{K}_N^{N'}$ may be calculated efficiently by the procedure in Sec. II F of I, with a change of definition of $\tilde{\varepsilon}_n$ as

$$\tilde{\varepsilon}_n \equiv \left(|\varepsilon_n| + \frac{1}{2\tau}\right){\rm sgn}(\varepsilon_n). \tag{23}$$

C. Analytic results at $T=0$

Now it will be shown that Eqs. (14a) and (14b) reduce to an identical expression at $T=0$ for arbitrary impurity concentrations, which has the physical meaning of the zero-energy density of states.

Let us start from Eq. (14a) where $\varepsilon_n>0$ and $\varepsilon_n<0$ yield the same contribution. Using this fact and Eq. (18a), it is transformed into

$$\frac{S_{\rm s}}{S_{\rm n}} = 1 - \frac{3\Delta_0^2}{2\pi^2T^2}\left[1 - 2\pi T\sum_{n=0}^{\infty}\left(\langle \tilde{f}_0^{(1)}\rangle + \varepsilon_n \frac{\partial \langle \tilde{f}_0^{(1)}\rangle}{\partial \varepsilon_n}\right)\right]. \tag{24}$$

The summation over n for $T\to 0$ may be performed by using the Euler-Maclaurin formula and the asymptotic property $\tilde{f}_0^{(1)}(\varepsilon_n) \to \varepsilon_n^{-1}$ $(\varepsilon_n\to\infty)$.[14] For example,

$$\begin{aligned} 2\pi T\sum_{n=0}^{\infty}\langle \tilde{f}_0^{(1)}(\varepsilon_n)\rangle &\approx \int_{\pi T}^{\infty}\langle \tilde{f}_0^{(1)}(\varepsilon)\rangle\, d\varepsilon + \pi T\langle \tilde{f}_0^{(1)}(\pi T)\rangle \\ &\quad - \frac{(\pi T)^2}{3}\langle \tilde{f}_0^{(1)\prime}(\pi T)\rangle \\ &\approx \int_0^{\infty}\langle \tilde{f}_0^{(1)}(\varepsilon)\rangle\, d\varepsilon + \frac{(\pi T)^2}{6}\langle \tilde{f}_0^{(1)\prime}(0)\rangle. \end{aligned} \tag{25}$$

We thereby obtain

$$\frac{S_{\rm s}}{S_{\rm n}} \overset{T\to 0}{\longrightarrow} 1 + \frac{\Delta_0^2}{2}\langle \tilde{f}_0^{(1)\prime}(0)\rangle. \tag{26a}$$

Equation (14b) may be transformed similarly as

$$\frac{M_{\rm sP}}{M_{\rm nP}} = 1 - \pi T\Delta_0^2\sum_{n=0}^{\infty}\frac{\partial^2\langle \tilde{f}_0^{(1)}(\varepsilon_n)\rangle}{\partial \varepsilon_n^2} \overset{T\to 0}{\longrightarrow} 1 + \frac{\Delta_0^2}{2}\langle \tilde{f}_0^{(1)\prime}(0)\rangle. \tag{26b}$$

Thus, $S_{\rm s}/S_{\rm n} = M_{\rm sP}/M_{\rm nP}$, or equivalently, $\alpha_S=\alpha_\chi$ at $T=0$ for arbitrary impurity concentrations.

Equations (26a) and (26b) have a simple physical meaning. Indeed, noting Eqs. (11), (13b), and (18a), we find an alternative expression at $T=0$:

$$\frac{S_{\rm s}}{S_{\rm n}} = \frac{M_{\rm sP}}{M_{\rm nP}} = \frac{1}{V}\int \langle g(\varepsilon_n=0,\mathbf{k}_{\rm F},\mathbf{r})\rangle d\mathbf{r}, \tag{27}$$

which is nothing but the normalized density of states at $\varepsilon=0$. Thus, the entropy and the spin susceptibility at $T=0$ are both determined by the zero-energy density of states.

The coefficient of $\Delta_0^2 \propto H_{c2}-B$ have been obtained in I. Also, $\tilde{f}_0^{(1)\prime}(0)$ in Eqs. (26a) and (26b) may be calculated efficiently from Eq. (22) by using the analytic expression[14]

$$\tilde{K}_0^0(\tilde{\varepsilon}_n,\beta) = \sqrt{\frac{2}{\pi}}\int_0^{\infty}\frac{\tilde{\varepsilon}_n}{\tilde{\varepsilon}_n^2 + x^2\beta^2}e^{-x^2/2}\,dx, \tag{28}$$

with $\beta \equiv \sqrt{H_{c2}}\sin\theta/2\sqrt{2}$. Hence, Eqs. (26a) and (26b) at $T=0$ can be evaluated easily.

D. Analytic results in the dirty limit

I here summarize analytic results in the dirty limit $\tau\to 0$. First, the key quantities $\tilde{K}_N^0$ are calculated by choosing $N_{\rm cut}=1$ in the procedure in Sec. II F of I. The results are given by

$$\tilde{K}_0^0 = \frac{\tilde{\varepsilon}_n}{\tilde{\varepsilon}_n^2+\beta^2}, \quad \tilde{K}_1^0 = \frac{\beta}{\tilde{\varepsilon}_n^2+\beta^2}. \tag{29}$$

Since β^2 is of the order of $1/\tau$, as shown below, $\langle \tilde{K}_0^0\rangle$ may be approximated as $\langle \tilde{K}_0^0\rangle \approx \langle 1/\tilde{\varepsilon}_n - \beta^2/\tilde{\varepsilon}_n^3\rangle \approx \tilde{\varepsilon}_n/(\tilde{\varepsilon}_n^2 + \langle\beta^2\rangle)$. Using this $\langle \tilde{K}_0^0\rangle$ in Eq. (22) and retaining only the leading-order contributions, we obtain

$$\tilde{f}_0^{(1)} = \frac{1}{|\varepsilon_n| + 2\tau\langle\beta^2\rangle}, \quad \tilde{f}_1^{(1)} = \frac{2\tau\beta\,{\rm sgn}(\varepsilon_n)}{|\varepsilon_n| + 2\tau\langle\beta^2\rangle}. \tag{30}$$

Notice that $\tilde{f}_1^{(1)}$ is smaller than $\tilde{f}_0^{(1)}$ by $\sqrt{\tau}$. Substitution of Eq. (30) into Eq. (15) leads to the equation for H_{c2} obtained by Maki[28] and de Gennes[29]:

$$\ln(T_c/T) + \psi(1/2) - \psi(x) = 0, \tag{31}$$

where ψ is the digamma function, and x is defined by

$$x \equiv \frac{1}{2} + \frac{\tau\langle\beta^2\rangle}{\pi T} = \frac{1}{2} + \frac{\tau H_{c2}}{4\pi T d}, \tag{32}$$

with $d=2,3$ the dimension of the system. As shown by Maki,[28] Eq. (31) can be solved near $T=0$ by using the asymptotic expression of $\psi(x)$ as

$$H_{c2} \approx \frac{d}{\tau}\left[1 - \frac{2}{3}(\pi T)^2\right]. \tag{33}$$

Thus $\beta^2 \propto H_{c2} \sim \tau^{-1}$, as assumed at the beginning. Differentiating Eq. (31) with respect to T, we obtain

$$\frac{dH_{c2}}{dT}=\frac{H_{c2}}{T}\left[1-\frac{4\pi Td}{\tau H_{c2}\psi'(x)}\right]. \tag{34}$$

Finally, κ_2 and $[\Delta_0(B)]^2$ are calculated from Eqs. (34b) and (36) of I as

$$\kappa_2=\frac{d\sqrt{-\psi^{(2)}(x)}}{\sqrt{2}\tau\psi'(x)}\kappa_0\overset{T\to 0}{\to}\frac{H_{c2}}{\sqrt{2}}\kappa_0, \tag{35}$$

$$\Delta_0^2=\frac{(H_{c2}-B)\kappa_0^2}{(2\kappa_2^2-1)\beta_A+1}\,\frac{4\pi Td}{\tau\psi'(x)}\overset{T\to 0}{\to}\frac{(H_{c2}-B)H_{c2}\kappa_0^2}{(H_{c2}^2\kappa_0^2-1)\beta_A+1}, \tag{36}$$

where κ_0 is defined by $\kappa_0\equiv\phi_0/2\pi\xi_0^2H_c(0)$ with $H_c(0)$ the thermodynamic critical field at $T=0$. Equation (35) agrees with the result by Caroli, Cyrot, and de Gennes.[30]

Now, let us substitute Eq. (30) into Eqs. (14b) and (19) and use Eq. (33). We thereby obtain

$$\frac{S_s}{S_n}=1+\frac{dH_{c2}}{dT}\,\frac{3\tau\Delta_0^2}{8\pi^3T^2d}\psi'(x)\overset{T\to 0}{\to}1-2\Delta_0^2, \tag{37a}$$

$$\frac{M_{sP}}{M_{nP}}=1+\frac{\Delta_0^2}{8\pi^2T^2}\psi^{(2)}(x)\overset{T\to 0}{\to}1-2\Delta_0^2. \tag{37b}$$

Thus, M_{sP}/M_{nP} and S_s/S_n are the same at $T=0$, in agreement with Eq. (27); they are both determined by the zero-energy density of states. Equation (37b) is the result first obtained by Maki.[2] Also, the expression $1-2\Delta_0^2$ for the normalized zero-energy density of states at $T=0$ agrees with the result for the local density of states by de Gennes.[4,29]

Equation (36) tells us that $\Delta_0^2=(1-B/H_{c2})\beta_A^{-1}$ as $T\to 0$ for $\kappa_2\gg 1$. We hence find from Eqs. (1), (37a), and (37b) that the initial slopes at $T=0$ for $\kappa_2\gg 1$ are given by

$$\alpha_S=\alpha_\chi=2/\beta_A=1.72. \tag{38}$$

The results suggest the overall field dependence of S_s and χ_s at $T=0$ which is convex downward. Notice that the flux-flow resistivity ρ_f at $T=0$ also has the same initial slope $\alpha_\rho=1.72$ in the dirty limit.[15,31,32] These results strongly suggest that the density of states at $\varepsilon=0$ is mainly relevant to the physical properties of the vortex state at $T=0$.

E. The case with *p*-wave impurity scattering

If the *p*-wave impurity scattering is relevant, the following additional terms appear on the right-hand side of Eq. (5):

$$d\frac{f\hat{\mathbf{k}}\cdot\langle\hat{\mathbf{k}}'f^\dagger\rangle+\langle f\hat{\mathbf{k}}'\rangle\cdot\hat{\mathbf{k}}f^\dagger}{4\tau_1}+d\frac{g\hat{\mathbf{k}}\cdot\langle\hat{\mathbf{k}}'g\rangle}{2\tau_1}, \tag{39}$$

where $\langle\hat{\mathbf{k}}'g\rangle\equiv\langle\hat{\mathbf{k}}'g(\varepsilon_n,\mathbf{k}_F',\mathbf{r})\rangle$, for example, τ_1 is the *p*-wave relaxation time, and $\hat{\mathbf{k}}$ is the unit vector along $\mathbf{k}_F$. However, Eqs. (7), (9), and (10) remain unchanged once I is modified as above.

The corresponding calculations near H_{c2} may be performed as described in Appendix A of I. It thereby follows that Eqs. (14) and (21) are also valid together with Eqs. (17), (18a), and (20), where $\tilde{f}_N^{(1)}$ is now given by

$$\tilde{f}_N^{(1)}=\frac{1}{D}\left\{\left[1-\frac{d}{4\tau_1}\langle\tilde{K}_1^1\sin^2\theta'\rangle\mathrm{sgn}(\varepsilon_n)\right]\tilde{K}_N^0\,\mathrm{sgn}(\varepsilon_n)+\frac{d}{4\tau_1}\langle\tilde{K}_1^0\sin\theta'\rangle\tilde{K}_N^1\sin\theta\right\}, \tag{40}$$

with

$$D\equiv\left[1-\frac{1}{2\tau}\langle\tilde{K}_0^0\rangle\mathrm{sgn}(\varepsilon_n)\right]\left[1-\frac{d}{4\tau_1}\langle\tilde{K}_1^1\sin^2\theta'\rangle\mathrm{sgn}(\varepsilon_n)\right]+\frac{d}{8\tau\tau_1}\langle\tilde{K}_1^0\sin\theta'\rangle^2. \tag{41}$$

In addition, Eq. (18b) is to be replaced by

$$\frac{\partial\tilde{f}_N^{(1)}}{\partial\varepsilon_n}=-\sum_{N}\tilde{K}_N^{N'}\tilde{f}_{N'}^{(1)}+\frac{\tilde{K}_N^0}{2\tau}\mathrm{sgn}(\varepsilon_n)\frac{\partial\langle\tilde{f}_0^{(1)}\rangle}{\partial\varepsilon_n}+d\frac{\tilde{K}_N^1\sin\theta}{4\tau_1}\mathrm{sgn}(\varepsilon_n)\frac{\partial\langle\tilde{f}_1^{(1)}\sin\theta'\rangle}{\partial\varepsilon_n}, \tag{42}$$

where

$$\frac{\partial\langle\tilde{f}_0^{(1)}\sin\theta'\rangle}{\partial\varepsilon_n}=-\sum_N(-1)^N\langle\tilde{f}_N^{(1)}\tilde{\phi}_N^{(1)}\rangle\mathrm{sgn}(\varepsilon_n), \tag{43}$$

with

$$\tilde{\phi}_N^{(1)}\equiv\frac{1}{D}\left\{-\left[1-\frac{1}{2\tau}\langle\tilde{K}_0^0\rangle\mathrm{sgn}(\varepsilon_n)\right]\tilde{K}_N^1\sin\theta\,\mathrm{sgn}(\varepsilon_n)+\frac{1}{2\tau}\langle\tilde{K}_1^0\sin\theta'\rangle\tilde{K}_N^0\right\}. \tag{44}$$

Finally, the analytic results in the dirty limit are the same as those given in Sec. II D with a replacement of τ by the transport lifetime τ_{tr} defined through

$$\frac{1}{\tau_{tr}}\equiv\frac{1}{\tau}-\frac{1}{\tau_1}. \tag{45}$$

F. Numerical procedures

I have adopted the same parameters as I and II to express different impurity concentrations:

$$\xi_E/l_{tr}\equiv 1/2\pi T_c\tau_{tr},\quad l_{tr}/l\equiv\tau_{tr}/\tau. \tag{46}$$

Numerical calculations of Eqs. (14) and (21) with Eqs. (17), (18), and (20) have been performed for each set of parameters by restricting every summation over the Matsubara frequencies to those satisfying $|\varepsilon_n|\leqslant\varepsilon_c$. Choosing $\varepsilon_c=200$ is sufficient to obtain an accuracy of ~0.1% for Eqs. (14b) and (21), whereas $\varepsilon_c=20\,000$ (4000) is required for Eq. (14a) in the dirty (clean) limit. Summations over Landau levels have been truncated at $N=N_{cut}$ where I put $\mathcal{R}_{N_{cut}}=1$ in the calculation of $\tilde{K}_N^{N'}$; see Sec. II F of I for the details. Enough

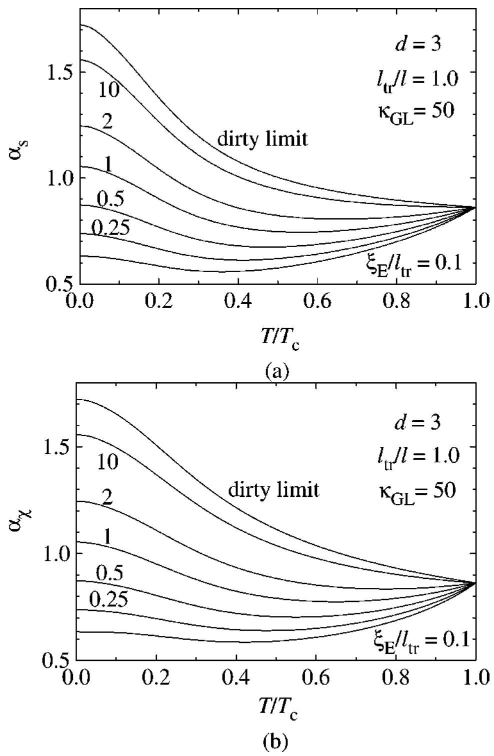

FIG. 1. Slopes (a) α_S and (b) α_χ near H_{c2} as a function of T/T_c for different impurity concentrations with $d=3$, $l_{tr}/l=1.0$, and $\kappa_{GL}=50$.

convergence has been obtained by choosing $N_{cut}=4$, 40, 100, 200, 1500, and 4000 for $\xi_E/l_{tr}=50$, 1.0, 0.5, 0.1, and 0.05, respectively. Finally, integrations over θ have been performed by Simpson's formula with $N_{cut}+1$ integration points for $0 \leqslant \theta \leqslant \pi/2$.

III. RESULTS

Figure 1 shows temperature dependence of α_S and α_χ defined by Eqs. (1a) and (1b), respectively, for different impurity concentrations parametrized by Eq. (46). They have been calculated in three dimensions for $l_{tr}/l=1.0$ and $\kappa_{GL}=50$, where κ_{GL} is the Ginzburg-Landau parameter.[33] All the curves start from the same value $\alpha_S=\alpha_\chi=0.862$ at $T=T_c$ and develop differences among different impurity concentrations at lower temperatures. The equality $\alpha_S=\alpha_\chi$ holds at $T=0$, as shown by Eq. (27), and the value decreases from 1.72 in the dirty limit to around 0.6 for $\xi_E/l_{tr}=0.1$. According to Eq. (27), this variation in the slope at $T=0$ can be attributed to the mean-free-path dependence of the zero-energy density of states $N_s(0,B)$. In particular, $N_s(0,B)$ in the dirty (clean) limit decreases more rapidly (mildly) than the linear behavior $N(0)B/H_{c2}$ near H_{c2}. From this result, we expect the overall field dependence of the entropy and the spin susceptibility at $T=0$ which is convex downward (upward) in the dirty (clean) limit, as seen from Eq. (1).

The difference between α_S and α_χ at finite temperatures is small, as expected from $\alpha_S=\alpha_\chi$ holding at $T=0$ and T_c. In particular, the curves of α_S and α_χ in the dirty limit depend neither on the dimensions nor l_{tr}/l. However, the dependence develops gradually as the mean free path becomes longer.

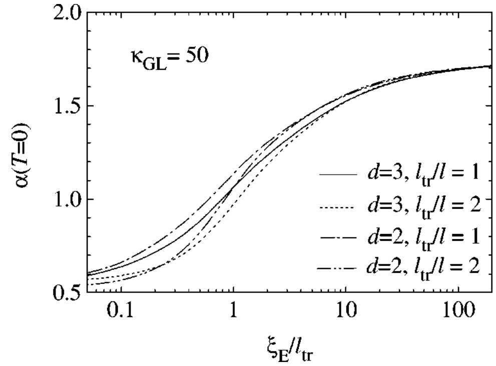

FIG. 2. Slope $\alpha(T=0)\equiv\alpha_S(T=0)=\alpha_\chi(T=0)$ as a function of ξ_E/l_{tr} for $d=2,3$, $l_{tr}/l=1,2$, and $\kappa_{GL}=50$.

Figure 2 shows the slope $\alpha\equiv\alpha_S=\alpha_\chi$ at $T=0$ as a function of ξ_E/l_{tr} for different combinations of dimensions and impurity scatterings. The four curves start from the same value 1.72 in the dirty limit, and decrease gradually through unity towards 0.5–0.6 in the clean limit. However, we observe only small dependence of $\alpha(T=0)$ on d and l_{tr}/l. We thus realize that the zero-energy density of states is mainly determined by the mean free path, and may not depend much on the Fermi-surface structures nor the details of the impurity scattering.

For comparison, Fig. 3 presents the slope α_ρ for the flux-flow resistivity ρ_f calculated previously[15] for the same parameters as in Fig. 1. At finite temperatures in the dirty limit, α_ρ is much larger than α_S and α_χ, indicating a steeper decrease of ρ_f just below H_{c2}. However, the difference is seen to diminish as the temperature is reduced, and it has been checked numerically that $\alpha_S=\alpha_\chi=\alpha_\rho$ holds at $T=0$ for arbitrary impurity concentrations. This fact suggests that ρ_f at $T=0$ is also determined by the zero-energy density of states.

Next, we examine the dependence of the slopes on the Ginzburg-Landau parameter κ_{GL}. Figure 4 shows the same curves as in Fig. 1 near the type-I–type-II boundary of $\kappa_{GL}=1$. Each curve is shifted upwards from the corresponding one in Fig. 1 for $\kappa_{GL}=50$, but the quantitative difference is

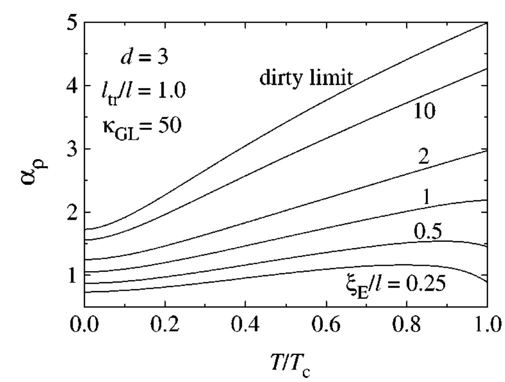

FIG. 3. Slope α_χ for the flux-flow resistivity near H_{c2} as a function of T/T_c for different impurity concentrations, with $d=3$, $l_{tr}/l=1.0$, and $\kappa_{GL}=50$.

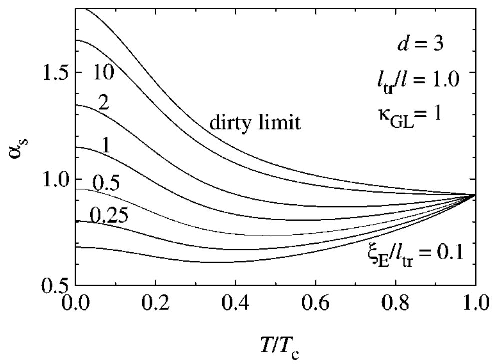

FIG. 4. Slope α_S as a function of T/T_c for different impurity concentrations with $d=3$, $l_{tr}/l=1.0$, and $\kappa_{GL}=1$.

rather small. This is also the case for α_χ. Thus, the slopes α_S and α_χ defined in terms of B do not have large κ_{GL} dependence.

Finally, Fig. 5 plots the specific-heat jump ΔC over T at H_{c2} as a function of T/T_c for different impurity concentrations with $d=3$, $l_{tr}/l=1$, and $\kappa_{GL}=50$. It is normalized by the corresponding quantity at $T=T_c$ and $H=0$, i.e., $\Delta C(T_c)/T_c=1.43$ in the weak-coupling model. The curves change gradually from almost T-linear overall temperature dependence in the dirty limit to T^2 dependence in the clean limit, and approach zero as $\propto T^2$ at lowest temperatures.[1] Although the ratio near T_c is strongly dependent on κ_{GL} as[12]

$$\lim_{T_{cH}\to T_c} \frac{\Delta C(T_{cH})/T_{cH}}{\Delta C(T_c)/T_c} = \frac{2\kappa_{GL}^2}{(2\kappa_{GL}^2-1)\beta_A}, \tag{47}$$

the basic features mentioned above are common among different values of κ_{GL}, $d=2,3$, and $l_{tr}/l=1,2$.

IV. SUMMARY

The entropy and the spin susceptibility near H_{c2} have been calculated for *s*-wave type-II superconductors with arbitrary impurity concentrations. The results have been expressed conveniently with respect to the initial slopes α_S and α_χ defined by Eq. (1). The main conclusions are summarized as follows: (i) $\alpha_S=\alpha_\chi$ holds both at $T=0$ and $T=T_c$. (ii) $\alpha_S=\alpha_\chi=0.862$ at $T=T_c$ for all impurity concentrations. (iii) At $T=0$, the slope α decreases from 1.72 in the dirty limit to

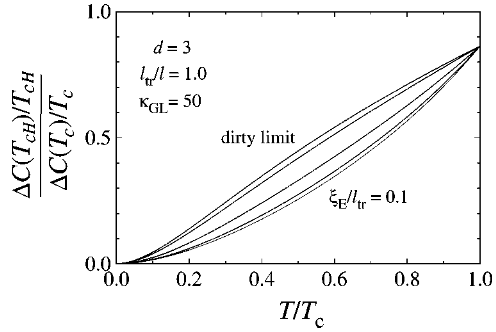

FIG. 5. Specific-heat jump divided by T at H_{c2}, normalized by the corresponding quantity at $T=T_c$ and $H=0$, as a function of T/T_c with $d=3$, $l_{tr}/l=1$, and $\kappa_{GL}=50$. The curves are for $\xi_E/l_{tr}=\infty$, 10, 1, 0.25, and 0.1 from the top to the bottom.

0.5–0.6 in the clean limit. This change is due completely to the mean-free-path dependence of the zero-energy density of states. The fact also suggests variation of the overall field dependence at $T=0$ from convex downward in the dirty limit to upward in the clean limit. (iv) The slopes have only small dependence on the dimensions and the details of the impurity scattering. (v) The slope α_ρ for the flux-flow resistivity ρ_f, which has been calculated previously,[15] also shows a complete numerical agreement at $T=0$ with α_S and α_χ. This fact indicates that the zero-energy density of states is also responsible for ρ_f at $T=0$.

The T-linear specific-heat coefficient $\gamma_s(B)$ observed in clean materials[7–13] presents curves with $\alpha<1$, which is in a qualitative agreement with the present calculation. On the other hand, $\gamma_s(B)$ for dirty samples[8,10] follows the well-accepted linear field dependence $\propto B/H_{c2}$ and apparently in contradiction with the present result in the dirty limit. However, it should be noted that a careful experiment[34] on ρ_f shows field dependence near $T=0$ which is convex downward, and experimentally obtained α_ρ agrees quantitatively with the dirty-limit theory.[15,31,32] Detailed experiments on the mean-free-path dependence of $\gamma_s(B)$ and $\rho_f(B)$ are desired to remove these discrepancies.

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