Calculation of $\kappa_2(T)$ for *s*-wave type-II superconductors

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This paper presents revised calculations for the Maki parameters κ_1 and κ_2 and the pair potential $\Delta(\mathbf{r})$ of *s*-wave type-II superconductors near the upper critical field H_{c2} with arbitrary impurity concentration. It is found that Eilenberger's well-known results on κ_2 [Phys. Rev. **153**, 584 (1967)] are not correct quantitatively, which are modified appropriately. Calculations are also performed for a two-dimensional system with an isotropic Fermi surface. The results on clean systems differ substantially from those for the three-dimensional system with a spherical Fermi surface. This fact indicates the necessity of considering detailed Fermi-surface structures for a quantitative understanding of the parameters. The coefficient of $\Delta(\mathbf{r})\propto(H_{c2}-B)^{1/2}$, which is basic to any theoretical evaluation of the thermodynamic and transport properties near H_{c2}, is obtained accurately.

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I. INTRODUCTION

Following the preceding studies,[1–11] Eilenberger[12] performed an extensive calculation of the parameters $\kappa_1(T)$ and $\kappa_2(T)$ introduced by Maki[2] to distinguish temperature dependences of the upper critical field H_{c2} and the initial slope of the magnetization $\partial M/\partial H$, respectively. Based on the *s*-wave pairing with a spherical Fermi surface and taking both *s*- and *p*-wave impurity scatterings into account, he clarified a basic feature that $\kappa_2 \geqslant \kappa_1 \geqslant \kappa_{\rm GL}$, where $\kappa_{\rm GL}$ is the Ginzburg-Landau parameter near T_c.[13,14] He also found a large dependence of the parameters on the *p*-wave scattering strength. This study is undoubtedly one of the basic works in the field and has been referred to frequently in analyzing experimental results on the quantities. It will be shown, however, that his results on κ_2 are not correct quantitatively due to a couple of inappropriate approximations adopted.

This fact also tells us that we are still far from a quantitative description of type-II superconductors. The parameter κ_2 is such a basic quantity that it is relevant to all thermodynamic and transport properties near H_{c2}. Indeed, changes of those quantities through H_{c2} are proportional to the spatial average $\langle|\Delta(\mathbf{r})|^2\rangle$ of the pair potential $\Delta(\mathbf{r})$, and $\langle|\Delta(\mathbf{r})|^2\rangle$ is directly connected with κ_2, as seen below. Thus, an absence of a reliable theory on κ_2 also implies no quantitative theories for all the other quantities near H_{c2}. The exact limiting behaviors would be useful not only for their own sake, but also for getting an insight into the behaviors over $0 \leqslant B \leqslant H_{c2}$. In addition, they would serve as a guide for any detailed numerical studies for $0 \leqslant B \leqslant H_{c2}$.

With these observations, I here perform revised calculations for the Maki parameters and the pair potential near H_{c2}. Besides correcting Eilenberger's results on κ_2 for the spherical Fermi surface, I also perform two-dimensional calculations of the quantities for an isotropic (i.e., cylindrical or circle) Fermi surface. Thereby clarified will be a rather large dependence of $\kappa_1(T)$ and $\kappa_2(T)$ on detailed Fermi-surface structures. Indeed, even the empirical inequality $\kappa_2 \geqslant \kappa_1 \geqslant \kappa_{\rm GL}$ will be shown violated in some cases for the two dimensions, even without the spin paramagnetism.[11]

The starting point adopted for these purposes is the quasiclassical Eilenberger equations.[15] As emphasized by Eilenberger[15] and also by Serene and Rainer,[16] the quasiclassical equations have an advantage over Gor'kov equations[17] that they are easier to solve due to the absence of an irrelevant energy variable. They have a rigorous microscopic foundation and hence form a firm basis for any quantitative description of superconducting/superfluid Fermi liquids.[16] Thus, it seems somewhat surprising that few calculations on κ_2 have been performed based on the Eilenberger equations.[18]

This paper is organized as follows. Section II provides the formulation for the *s*-wave pairing with an isotropic Fermi surface and *s*-wave impurity scattering, deferring *p*-wave impurity scattering to Appendix B. The main results are given in Secs. II E and II F, and the differences from Eilenberger's calculation are explained in Sec. II H. Section III presents numerical results. Section IV summarizes the paper, with possible extensions to include realistic Fermi surfaces from first-principles calculations and/or anisotropic pairings. Appendix A derives an analytic expression for the magnetization.

II. FORMULATION

A. Eilenberger equations

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 vector potential in the bulk can be written as[19–24]

$$\mathbf{A}(\mathbf{r}) = Bx\hat{\mathbf{y}} + \tilde{\mathbf{A}}(\mathbf{r}), \tag{1}$$

where B is the average flux density produced jointly by the external current outside the sample and the supercurrent inside it, 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 adopt the units 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. I also put $\hbar = k_{\mathrm{B}} = 1$ and use the gauge where $\boldsymbol{\nabla}\cdot\tilde{\mathbf{A}} = 0$. The Eilenberger equations[15] now read

$$\left[\varepsilon_n + \frac{\langle g\rangle}{2\tau} + \frac{\hat{\mathbf{v}}}{2}\cdot(\boldsymbol{\nabla} - i\mathbf{A})\right] f = \left(\Delta + \frac{\langle f\rangle}{2\tau}\right) g, \tag{2a}$$

$$\Delta(\mathbf{r})\ln\frac{T_c}{T} = -2\pi T\sum_{n=0}^{\infty}\left[\langle f(\varepsilon_n, \mathbf{k}_{\mathrm{F}}, \mathbf{r})\rangle - \frac{\Delta(\mathbf{r})}{\varepsilon_n}\right], \tag{2b}$$

$$-\nabla^2 \tilde{\mathbf{A}}(\mathbf{r}) = -\frac{i}{\kappa_0^2} 2\pi T \sum_{n=0}^{\infty} \langle \hat{\mathbf{v}} g(\varepsilon_n, \mathbf{k}_{\mathrm{F}}, \mathbf{r})\rangle. \tag{2c}$$

Here ε_n is the Matsubara frequency, τ is the relaxation time in the second-Born approximation, $\langle \cdots \rangle$ denotes the Fermi-surface average satisfying $\langle 1\rangle = 1$, $\Delta(\mathbf{r})$ is the pair potential, and the unit vector $\hat{\mathbf{v}} = \hat{\mathbf{k}}$ specifies a point on the isotropic Fermi surface. The quasiclassical Green's functions f and g are connected by $g = (1 - ff^{\dagger})^{1/2}$ with $f^{\dagger}(\varepsilon_n, \mathbf{k}_{\mathrm{F}}, \mathbf{r}) \equiv f^*(\varepsilon_n, -\mathbf{k}_{\mathrm{F}}, \mathbf{r})$, and the dimensionless parameter κ_0 is defined by

$$\kappa_0 \equiv \phi_0/2\pi\xi_0^2 H_c(0), \tag{3}$$

where $H_c(0) \equiv \sqrt{4\pi N(0)}\Delta(0)$ is the thermodynamic critical field at $T=0$ with $N(0)$ the density of states per spin and per unit volume. Equations (2a)–(2c) are to be solved self-consistently for a fixed B. Finally, the missing connection between H and B is obtained by applying the Doria-Gubernatis-Rainer scaling[25] to Eilenberger's free-energy functional.[15] The details are given in Appendix A. The final result is given by

$$H = B + \frac{1}{BV}\int d\mathbf{r}\,(\boldsymbol{\nabla}\times\tilde{\mathbf{A}})^2 + \frac{\pi T}{2BV\kappa_0^2}\sum_{n=0}^{\infty}\int d\mathbf{r}\left\langle \frac{f^{\dagger}\hat{\mathbf{v}}\cdot(\boldsymbol{\nabla} - i\mathbf{A})f - f\hat{\mathbf{v}}\cdot(\boldsymbol{\nabla} + i\mathbf{A})f^{\dagger}}{1+g}\right\rangle, \tag{4}$$

where V is the volume of the system.

B. Expansion near H_{c2}

Near H_{c2}, the coupled equations (2) and (4) are expanded in terms of $\Delta(\mathbf{r})$ as follows. First, let us rewrite[24]

$$\frac{\hat{\mathbf{v}}}{2}\cdot(\boldsymbol{\nabla} - i\mathbf{A}) = \frac{\sqrt{B}\sin\theta}{2\sqrt{2}}[e^{-i\varphi}(a + \tilde{A}) - e^{i\varphi}(a^{\dagger} + \tilde{A}^*)], \tag{5}$$

where (θ, φ) are the polar angles of $\hat{\mathbf{v}}$, and the quantities a, $a^{\dagger}$, and $\tilde{A}$ are defined by

$$a \equiv \frac{1}{\sqrt{2B}}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} + Bx\right),$$

$$a^{\dagger} \equiv \frac{1}{\sqrt{2B}}\left(-\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} + Bx\right), \tag{6a}$$

$$\tilde{A} \equiv -i\frac{\tilde{A}_x + i\tilde{A}_y}{\sqrt{2B}}, \tag{6b}$$

with $[a, a^{\dagger}] = 1$. The operators $(a, a^{\dagger})$ are the same as (a_-, a_+) introduced by Helfand and Werthamer,[5] and (F_-, F_+) by Eilenberger.[12]

I then expand f, g, and $\tilde{A}$ up to the third order in $\Delta(\mathbf{r})$ as

$$f = f^{(1)} + f^{(3)},$$

$$g = 1 - \frac{1}{2} f^{(1)\dagger} f^{(1)},$$

$$\tilde{A} = \tilde{A}^{(2)}. \tag{7}$$

Substituting Eqs. (5) and (7) into Eq. (2a) and collecting terms of the same orders, we obtain

$$[\tilde{\varepsilon}_n + \beta(e^{-i\varphi}a - e^{i\varphi}a^{\dagger})] f^{(1)} = \Delta + \frac{\langle f^{(1)}\rangle}{2\tau}, \tag{8a}$$

$$\begin{aligned}
[\tilde{\varepsilon}_n + \beta(e^{-i\varphi}a - e^{i\varphi}a^{\dagger})] f^{(3)} &= \frac{\langle f^{(3)}\rangle}{2\tau} - \frac{f^{(1)\dagger}f^{(1)}}{2}\left(\Delta + \frac{\langle f^{(1)}\rangle}{2\tau}\right) \\
&\quad + \frac{\langle f^{(1)\dagger}f^{(1)}\rangle}{4\tau} f^{(1)} \\
&\quad - \beta(e^{-i\varphi}\tilde{A}^{(2)} - e^{i\varphi}\tilde{A}^{(2)*}) f^{(1)},
\end{aligned} \tag{8b}$$

with

$$\tilde{\varepsilon}_n \equiv \varepsilon_n + \frac{1}{2\tau}, \quad \beta \equiv \frac{\sqrt{B}\sin\theta}{2\sqrt{2}}. \tag{9}$$

Also, Eq. (2b) is transformed into

$$\Delta(\mathbf{r})\ln\frac{T_c}{T} = -2\pi T\sum_{n=0}^{\infty}\left[\langle f^{(1)}\rangle + \langle f^{(3)}\rangle - \frac{\Delta(\mathbf{r})}{\varepsilon_n}\right]. \tag{10}$$

The Maxwell equation (2c) is given in the leading order by

$$-\nabla^2 \tilde{A}^{(2)} = \frac{\pi T}{\sqrt{2B}\kappa_0^2}\sum_n \langle f^{(1)\dagger} f^{(1)} e^{i\varphi}\sin\theta\rangle, \tag{11}$$

whereas Eq. (4) becomes

$$H - B = \frac{\pi T}{2\sqrt{2B}\kappa_0^2 V}\int d\mathbf{r}\sum_n \langle f^{(1)\dagger}(e^{-i\varphi}a - e^{i\varphi}a^{\dagger}) f^{(1)}\sin\theta\rangle. \tag{12}$$

C. Two-dimensional calculations

To investigate the dependence of the Maki parameters on the Fermi-surface structure, calculations will also be performed for a two-dimensional system with an isotropic Fermi surface placed in the xy plane perpendicular to $\mathbf{B}$. The analytic expressions for this case can be obtained from those of the three dimensions by simply putting $\sin\theta \to 1$ and omitting the integrations over θ.

D. Transformation into algebraic equations

Equations (8) and (10)–(12) are solved with the Landau-level expansion method[24] by expanding Δ, $f^{(\nu)}$ ($\nu=1,3$), and $\tilde{A}^{(2)}$ in terms of periodic basis functions of the flux-line lattice as

$$\Delta(\mathbf{r})=\sqrt{V}\sum_{N=0}^{\infty}\Delta_N\,\psi_{N\mathbf{q}}(\mathbf{r}), \tag{13a}$$

$$f^{(\nu)}(\varepsilon_n,\mathbf{k}_{\mathrm{F}},\mathbf{r})=\sqrt{V}\sum_{m=-\infty}^{\infty}\sum_{N=0}^{\infty}f_{mN}^{(\nu)}(\varepsilon_n,\theta)e^{im\varphi}\psi_{N\mathbf{q}}(\mathbf{r}), \tag{13b}$$

$$\tilde{A}^{(2)}(\mathbf{r})=\sum_{\mathbf{K}\neq\mathbf{0}}\tilde{A}_{\mathbf{K}}^{(2)}e^{i\mathbf{K}\cdot\mathbf{r}}. \tag{13c}$$

Here N denotes the Landau level, $\mathbf{q}$ is an arbitrary chosen magnetic Bloch vector characterizing the broken translational symmetry of the flux-line lattice and specifying the core locations, and $\mathbf{K}$ is a reciprocal-lattice vector of the magnetic Brillouin zone. See Ref. 24 for the explicit expressions of the basis functions $\psi_{N\mathbf{q}}(\mathbf{r})$; they are essentially equivalent to Eilenberger's $\psi_N(\mathbf{r}|\mathbf{r}_0)$[12] and reduce for $N=0$ to Abrikosov's solution for the Ginzburg-Landau equations near H_{c2}.[26] It only suffices to know the properties:

$$\langle\psi_{N\mathbf{q}}|\psi_{N'\mathbf{q}}\rangle=\delta_{NN'}, \tag{14a}$$

$$a\,\psi_{N\mathbf{q}}=\sqrt{N}\psi_{N-1\mathbf{q}}, \tag{14b}$$

$$a^{\dagger}\psi_{N\mathbf{q}}=\sqrt{N+1}\psi_{N+1\mathbf{q}}. \tag{14c}$$

On the other hand, the expansion in $\mathbf{K}$ in Eq. (13c) was introduced by Brandt[22] for solving the Ginzburg-Landau equations over $0\leqslant B\leqslant H_{c2}$. This expansion enables us to integrate the Maxwell equation appropriately so that $\int\boldsymbol{\nabla}\times\tilde{\mathbf{A}}d\mathbf{r}=\mathbf{0}$ is satisfied automatically.

Quite a simplification results in Eq. (13) near H_{c2} for the s-wave pairing with an isotropic Fermi surface. Indeed, $\Delta(\mathbf{r})$ can be described excellently with only the lowest Landau level as[24]

$$\Delta(\mathbf{r})=\sqrt{V}\Delta_0\psi_{0\mathbf{q}}(\mathbf{r}). \tag{15}$$

Equation (15) has a wide range of applicability over $B\gtrsim 0.1H_{c2}$ both near T_c and in the dirty limit. However, the region in the clean limit shrinks as $T\to 0$ to disappear eventually. It should also be noted that higher Landau levels of even N become relevant for anisotropic pairings and/or anisotropic Fermi surfaces at low temperatures.

Substituting Eqs. (13b), (13c), and (15) into Eq. (8) and using the orthogonality of $e^{im\varphi}$ and $\psi_{N\mathbf{q}}$, we realize that $f_{mN}^{(\nu)}$ can be written as

$$f_{mN}^{(\nu)}=\delta_{mN}\Delta_0^{\nu}\tilde{f}_N^{(\nu)}. \tag{16}$$

Equations (8) and (10)–(12) are thereby transformed into algebraic equations for $\tilde{f}^{(1)}$, $\tilde{f}^{(3)}$, Δ_0, $\tilde{A}_{\mathbf{K}}^{(2)}$, and $H-B$ as

$$\sum_{N'}\tilde{\mathcal{M}}_{NN'}\tilde{f}_{N'}^{(1)}=\delta_{N0}\left(1+\frac{\langle\tilde{f}_0^{(1)}\rangle}{2\tau}\right), \tag{17a}$$

$$\sum_{N'}\tilde{\mathcal{M}}_{NN'}\tilde{f}_{N'}^{(3)}=\delta_{N0}\frac{\langle\tilde{f}_0^{(3)}\rangle}{2\tau}+J_N^{(3)}+J_N^{(A)}, \tag{17b}$$

$$\ln\frac{T_c}{T}=-2\pi T\sum_{n=0}^{\infty}\left(\langle\tilde{f}_0^{(1)}\rangle+\langle\tilde{f}_0^{(3)}\rangle\Delta_0^2-\frac{1}{\varepsilon_n}\right), \tag{17c}$$

$$\tilde{A}_{\mathbf{K}}^{(2)}=-\frac{2\pi T\Delta_0^2}{\kappa_0^2K^2}\sum_{n=0}^{\infty}\sum_{N}\frac{J_N^{(2)}(\varepsilon_n)I_{N+1N}(\mathbf{K})}{\sqrt{N+1}}, \tag{17d}$$

$$H-B=\frac{2\pi T\Delta_0^2}{\kappa_0^2}\sum_{n=0}^{\infty}\sum_{N}J_N^{(2)}(\varepsilon_n). \tag{17e}$$

Here the matrix $\tilde{\mathcal{M}}$ is defined by

$$\tilde{\mathcal{M}}_{NN'}\equiv\delta_{NN'}\tilde{\varepsilon}_n+\delta_{N,N'-1}\beta\sqrt{N+1}-\delta_{N,N'+1}\beta\sqrt{N}, \tag{18}$$

and J_N's are given by

$$J_N^{(2)}\equiv\frac{(-1)^N}{B}\sqrt{N+1}\,\langle\tilde{f}_{N+1}^{(1)}\tilde{f}_N^{(1)}\beta\rangle, \tag{19a}$$

$$J_N^{(3)}\equiv-\frac{1}{2}\sum_{N'}(-1)^{N'}I_{NN'N+N'0}^{(4)}\tilde{f}_{N'}^{(1)}\tilde{f}_{N+N'}^{(1)}\left(1+\frac{\langle\tilde{f}_0^{(1)}\rangle}{2\tau}\right)+\frac{1}{4\tau}\sum_{N'}(-1)^{N'}I_{NN'N'N}^{(4)}\langle\tilde{f}_{N'}^{(1)}\tilde{f}_{N'}^{(1)}\rangle\tilde{f}_N^{(1)}, \tag{19b}$$

$$J_N^{(A)}\equiv-\frac{\beta}{\Delta_0^2}\sum_{\mathbf{K}\neq\mathbf{0}}[I_{N+1N}^{*}(\mathbf{K})\tilde{A}_{\mathbf{k}}^{(2)}\tilde{f}_{N+1}^{(1)}-I_{NN-1}(\mathbf{K})\tilde{A}_{\mathbf{k}}^{(2)*}\tilde{f}_{N-1}^{(1)}], \tag{19c}$$

with[24]

$$I_{N_1N_2N_3N_4}^{(4)}\equiv V\int\psi_{N_1\mathbf{q}}^{*}\psi_{N_2\mathbf{q}}^{*}\psi_{N_3\mathbf{q}}\psi_{N_4\mathbf{q}}d\mathbf{r}, \tag{20a}$$

$$I_{N_1N_2}(\mathbf{K})\equiv\int\psi_{N_1\mathbf{q}}^{*}\psi_{N_2\mathbf{q}}e^{-i\mathbf{K}\cdot\mathbf{r}}d\mathbf{r}. \tag{20b}$$

Equation (17a) tells us that $\tilde{f}_N^{(1)}$ is real; this fact has been used in writing down Eqs. (17b)–(17e). As for $\tilde{f}_N^{(3)}$, numerical calculations show that $I^{(4)}$'s appearing in Eq. (19b) are all real for the relevant hexagonal lattice, with

$$\beta_{\mathrm{A}}\equiv I_{0000}^{(4)}=1.16. \tag{21}$$

Also, $I_{N+1N}(\mathbf{K})$ can be transformed with partial integrations as

$$2I_{N+1N}(\mathbf{K})=\frac{1}{\sqrt{N+1}}\int (a^{\dagger}\psi_{N\mathbf{q}})^{*}\psi_{N\mathbf{q}}e^{-i\mathbf{K}\cdot\mathbf{r}}d\mathbf{r}$$

$$=\frac{\sqrt{N}}{\sqrt{N+1}}I_{NN-1}(\mathbf{K})+\frac{K_y-iK_x}{\sqrt{2B(N+1)}}I_{NN}(\mathbf{K})$$

$$=\frac{K_y-iK_x}{\sqrt{2B(N+1)}}\sum_{N_1=0}^{N} I_{N_1N_1}(\mathbf{K}). \tag{22}$$

Since $I_{NN}(\mathbf{K})$ is real, $J^{(A)}$ is also real from Eq. (17d), and so is $\tilde{f}_N^{(3)}$.

It is desirable for a later purpose to express $J^{(A)}$ in terms of $I^{(4)}$ rather than $I_{N+1N}(\mathbf{K})$. This can be performed by first substituting Eq. (17d) into Eq. (19c), and then using Eq. (22) and the identity $\Sigma_{\mathbf{K}\neq\mathbf{0}}e^{i\mathbf{K}\cdot(\mathbf{r}-\mathbf{r}')}=V\delta(\mathbf{r}-\mathbf{r}')-1$. The result is given by

$$J_N^{(A)}=\frac{\pi T\beta}{B\kappa_0^2}\sum_{n'=0}^{\infty}\sum_{N'} J_{N'}^{(2)}[\sqrt{N+1}\tilde{f}_{N+1}^{(1)}(\mathcal{I}_{NN'}-1)$$

$$-\sqrt{N}\tilde{f}_{N-1}^{(1)}(\mathcal{I}_{N-1N'}-1)], \tag{23}$$

where $\tilde{f}_{N\pm1}^{(1)}\equiv\tilde{f}_{N\pm1}^{(1)}(\varepsilon_n)$, $J_{N'}^{(2)}\equiv J_{N'}^{(2)}(\varepsilon_{n'})$ is given by Eq. (19a), and $\mathcal{I}_{NN'}$ is an average of $I^{(4)}$ defined by

$$\mathcal{I}_{NN'}\equiv\frac{1}{(N+1)(N'+1)}\sum_{N_1=0}^{N}\sum_{N_1'=0}^{N'} I^{(4)}_{N_1N_1'N_1'N_1}. \tag{24}$$

E. Solutions

We are now ready to solve Eqs. (17a) and (17b). To this end, let us define

$$\tilde{K}_N^{N'}\equiv(\tilde{\mathcal{M}}^{-1})_{NN'}=(-1)^{N+N'}\tilde{K}_{N'}^{N}, \tag{25}$$

where the second equality originates from $\tilde{\mathcal{M}}_{NN'}=(-1)^{N+N'}\tilde{\mathcal{M}}_{N'N}$. Then Eq. (17a) is transformed into

$$\tilde{f}_N^{(1)}=\tilde{K}_N^0\left(1+\frac{\langle\tilde{f}_0^{(1)}\rangle}{2\tau}\right). \tag{26}$$

Solving Eq. (26) self-consistently for $\langle\tilde{f}_0^{(1)}\rangle$ and substituting the result into Eq. (26), we obtain

$$\tilde{f}_N^{(1)}=\frac{\tilde{K}_N^0}{1-\langle\tilde{K}_0^0\rangle/2\tau}. \tag{27}$$

The denominator in Eq. (27) corresponds to the so-called "vertex correction." Equation (17b) for $\tilde{f}_N^{(3)}$ may be handled similarly. Using the symmetry $\tilde{K}_0^N=(-1)^N\tilde{K}_N^0$, we thereby arrive at the expression for the relevant quantity $\langle\tilde{f}_0^{(3)}\rangle$ in Eq. (17c) as

$$\langle\tilde{f}_0^{(3)}\rangle=\sum_N (-1)^N\langle\tilde{f}_N^{(1)}(J_N^{(3)}+J_N^{(A)})\rangle. \tag{28}$$

The quantity $\Sigma_N(-1)^N\langle\tilde{f}_N^{(1)}J_N^{(A)}\rangle$ in Eq. (28) may be transformed further by using Eqs. (23) and (19a) as

$$\sum_N (-1)^N\langle\tilde{f}_N^{(1)}(\varepsilon_n)J_N^{(A)}(\varepsilon_n)\rangle$$

$$=\frac{1}{\kappa_0^2}\sum_N J_N^{(2)}(\varepsilon_n)2\pi T\sum_{n'=0}^{\infty}\sum_{N'} J_{N'}^{(2)}(\varepsilon_{n'})(\mathcal{I}_{NN'}-1). \tag{29}$$

We next consider the self-consistency equation (17c) for the pair potential. Here, $\tilde{f}_N^{(1)}(B)$ is expanded in terms of the distance $H_{c2}-B$ from H_{c2} as

$$\tilde{f}_N^{(1)}(B)=\tilde{f}_N^{(1)}(H_{c2})-\tilde{f}_N^{(1)\prime}(H_{c2})(H_{c2}-H+H-B), \tag{30}$$

whereas the higher-order term $\tilde{f}_N^{(3)}$ is evaluated at H_{c2}. To find an explicit expression for $\tilde{f}_N^{(1)\prime}$ in Eq. (30), let us differentiate Eq. (17a) with respect to B:

$$\sum_{N'} \tilde{\mathcal{M}}_{NN'}\tilde{f}_{N'}^{(1)\prime}=\delta_{N0}\frac{\langle\tilde{f}_0^{(1)\prime}\rangle}{2\tau}-\frac{\beta}{2B}(\sqrt{N+1}\tilde{f}_{N+1}^{(1)}-\sqrt{N}\tilde{f}_{N-1}^{(1)}). \tag{31}$$

This equation can be solved in the same way as Eq. (17a) to yield

$$\langle\tilde{f}_0^{(1)\prime}\rangle=-\sum_N J_N^{(2)}, \tag{32}$$

where $J_N^{(2)}$ is defined by Eq. (19a). Let us substitute Eqs. (28)–(30) and (32) into Eq. (17c), replace $H-B$ by the right-hand side of Eq. (17e), and regard $H_{c2}-H$ as second order. Collecting first-order terms, we obtain the equation to fix the second-order transition point $H=H_{c2}$ as

$$\ln\frac{T_c}{T}=-2\pi T\sum_{n=0}^{\infty}\left[\langle\tilde{f}_0^{(1)}(\varepsilon_n)\rangle-\frac{1}{\varepsilon_n}\right]. \tag{33}$$

The third-order terms determine the pair potential Δ_0 and the magnetization $H-B$ as a function of $H_{c2}-H$ as

$$\Delta_0^2=\frac{H_{c2}-H}{\kappa_0^2S_4/S_2^2-S_A/S_2^2}\frac{\kappa_0^2}{S_2}, \tag{34a}$$

$$H-B=\frac{H_{c2}-H}{\kappa_0^2S_4/S_2^2-S_A/S_2^2}\equiv\frac{H_{c2}-H}{(2\kappa_2^2-1)\beta_{\mathrm{A}}}, \tag{34b}$$

where S_2, S_4, and S_A are defined by

$$S_2\equiv2\pi T\sum_{n=0}^{\infty}\sum_{N=0}^{\infty} J_N^{(2)}(\varepsilon_n), \tag{35a}$$

$$S_4\equiv-2\pi T\sum_{n=0}^{\infty}\sum_{N=0}^{\infty}(-1)^N\langle\tilde{f}_N^{(1)}(\varepsilon_n)J_N^{(3)}(\varepsilon_n)\rangle, \tag{35b}$$

$$S_A \equiv (2\pi T)^2 \sum_{n=0}^{\infty}\sum_{n'=0}^{\infty}\sum_{N=0}^{\infty}\sum_{N'=0}^{\infty} J_N^{(2)}(\varepsilon_n) J_{N'}^{(2)}(\varepsilon_{n'}) \mathcal{I}_{NN'}, \tag{35c}$$

with $\tilde{f}_N^{(1)}$, J_N, and $\mathcal{I}_{NN'}$ given by Eqs. (27), (19), and (24), respectively. All the quantities in Eq. (35) are to be evaluated at H_{c2}. The latter equality in Eq. (34b) defines the Maki parameter κ_2 with $\beta_A \equiv I_{0000}^{(4)} = 1.16$.

Equation (34) forms the main result of the paper, which is not only exact but also convenient for numerical calculations. An extension to include p-wave impurity scattering is carried out in Appendix B, where it is shown that Eq. (34) is still valid with the replacements of $\tilde{f}_N^{(1)}$ and $J_N^{(3)}$ by Eqs. (B8) and (B9), respectively.

Sometimes it is physically more meaningful to express Δ_0 as a function of B instead of H, because B is the real average field inside the bulk directly relevant to the spatial profile of the pair potential. It is obtained, without the replacement of $H-B$ mentioned above Eq. (33), as

$$\Delta_0^2 = \frac{H_{c2}-B}{\kappa_0^2 S_4/S_2^2 - S_A/S_2^2 + 1}\,\frac{\kappa_0^2}{S_2}. \tag{36}$$

F. Calculation of $\tilde{K}_N^{N'}$

The key quantity in Eq. (34) is $\tilde{K}_N^{N'}$ defined by Eq. (25), as may be seen from Eqs. (27), (19), and (35). An efficient algorithm to calculate them is obtained as follows.

Let us define $\mathcal{D}_N$ ($\bar{\mathcal{D}}_N$) for $N=0,1,2,\ldots$ as the determinant of the submatrix obtained by removing (retaining) the first N rows and columns of the tridiagonal matrix $\tilde{\mathcal{M}}$ of Eq. (18), namely,

$$\mathcal{D}_N \equiv \det\begin{bmatrix} \tilde{\varepsilon}_n & \sqrt{N+1}\,\beta & 0 & \cdots \\ -\sqrt{N+1}\beta & \tilde{\varepsilon}_n & \sqrt{N+2}\beta & \cdots \\ 0 & -\sqrt{N+2}\beta & \tilde{\varepsilon}_n & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{bmatrix}, \tag{37a}$$

$$\bar{\mathcal{D}}_N \equiv \det\begin{bmatrix} \tilde{\varepsilon}_n & \sqrt{1}\,\beta & \cdots & \cdots & \cdots \\ -\sqrt{1}\,\beta & \tilde{\varepsilon}_n & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \tilde{\varepsilon}_n & \sqrt{N-1}\,\beta \\ \cdots & \cdots & \cdots & -\sqrt{N-1}\,\beta & \tilde{\varepsilon}_n \end{bmatrix}. \tag{37b}$$

They satisfy

$$\mathcal{D}_{N-1} = \tilde{\varepsilon}_n \mathcal{D}_N + N\beta^2 \mathcal{D}_{N+1}, \tag{38a}$$

$$\bar{\mathcal{D}}_{N+1} = \tilde{\varepsilon}_n \bar{\mathcal{D}}_N + N\beta^2 \bar{\mathcal{D}}_{N-1}, \tag{38b}$$

as shown by expanding Eqs. (37a) and (37b) with respect to the first and the last row, respectively.[27] Then $\tilde{K}_N^{N'}$ for $N' \leqslant N$ is obtained by also using standard techniques to solve linear equations[27] as

$$K_N^{N'} = \beta^{N-N'} \sqrt{\frac{N!}{N'!}}\,\frac{\mathcal{D}_{N+1}\bar{\mathcal{D}}_{N'}}{\mathcal{D}_0}. \tag{39}$$

This algorithm can be put into a more convenient form in terms of

$$\mathcal{R}_N \equiv \tilde{\varepsilon}_n \mathcal{D}_{N+1}/\mathcal{D}_N, \tag{40a}$$

$$\bar{\mathcal{R}}_N \equiv \tilde{\varepsilon}_n \bar{\mathcal{D}}_{N-1}/\bar{\mathcal{D}}_N. \tag{40b}$$

They satisfy

$$\mathcal{R}_{N-1} = \frac{1}{1+Nb^2\mathcal{R}_N}, \tag{41a}$$

$$\bar{\mathcal{R}}_{N+1} = \frac{1}{1+Nb^2\bar{\mathcal{R}}_N}, \tag{41b}$$

with $\bar{\mathcal{R}}_1 = 1$ and

$$b \equiv \beta/\tilde{\varepsilon}_n. \tag{42}$$

Then $\tilde{K}_N^N$ and $\tilde{K}_N^{N'}$ for $N' < N$ are obtained by

$$\tilde{K}_0^0 = \mathcal{R}_0/\tilde{\varepsilon}_n, \tag{43a}$$

$$\tilde{K}_N^N = (\mathcal{R}_N/\bar{\mathcal{R}}_N)\tilde{K}_{N-1}^{N-1}, \tag{43b}$$

$$\tilde{K}_N^{N'} = \sqrt{N}\,b\,\mathcal{R}_N \tilde{K}_{N-1}^{N'}. \tag{43c}$$

Numerical calculations of $\mathcal{R}_N$ may be carried out by starting from $\mathcal{R}_{N_{\rm cut}} = 1$ for an appropriately chosen large $N_{\rm cut}$ and using Eq. (41a) to decrease N. One can check the convergence by increasing $N_{\rm cut}$. It turns out that $N_{\rm cut}=1$ is sufficient both near T_c and in the dirty limit, thereby reproducing the analytic results by Gor'kov[17] and Caroli, Cyrot, and de Gennes,[10] respectively. In contrast, $N_{\rm cut} \gtrsim 1000$ is required in the clean limit at low temperatures.

Noting that Eq. (33) with Eq. (27) should be equivalent to the equation for H_{c2} obtained by Helfand and Werthamer,[5] we get an alternative expression for $\tilde{K}_0^0$ as

$$\tilde{K}_0^0(\tilde{\varepsilon}_n,\beta) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{\tilde{\varepsilon}_n}{\tilde{\varepsilon}_n^2 + x^2\beta^2} e^{-x^2/2}\, dx. \tag{44}$$

The equivalence between Eqs. (43a) and (44) can also be checked numerically.

G. Expression of $\kappa_{\rm GL}$

Near T_c where $\beta \ll \tilde{\varepsilon}_n$ holds, we may choose $N_{\rm cut}=1$ in Eqs. (41)–(43) and expand the resulting expressions with respect to $\beta/\tilde{\varepsilon}_n$. This yields $\tilde{K}_0^0 \approx 1/\tilde{\varepsilon}_n - \beta^2/\tilde{\varepsilon}_n^3$ and $\tilde{K}_1^0$

$\approx\beta/\tilde{\varepsilon}_n^2$, so that Eq. (27) can be approximated by $\tilde{f}_0^{(1)}\approx 1/\varepsilon_n - (\beta^2\varepsilon_n+\langle\beta^2\rangle/2\tau)/\varepsilon_n^2\tilde{\varepsilon}_n^2$ and $\tilde{f}_1^{(1)}\approx\beta/\varepsilon_n\tilde{\varepsilon}_n$. Using these results in Eq. (35) and retaining only terms of the leading order in β, we obtain

$$S_2=\frac{1}{2d(\pi T_c)^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2(2n+1+1/2\pi\tau T_c)}, \tag{45a}$$

$$S_4=\frac{7\zeta(3)}{8(\pi T_c)^2}\beta_{\rm A}, \tag{45b}$$

$$S_A=S_2^2\beta_{\rm A}, \tag{45c}$$

where $d=2,3$ is the dimension of the system. Substituting Eq. (45) into Eq. (34b), we find the expression of $\kappa_{\rm GL}\equiv\kappa_2(T_c)$ as

$$\kappa_{\rm GL}=\frac{d\,\pi T_c\sqrt{7\zeta(3)}/2}{\sum_n[(2n+1)^2(2n+1+1/2\pi\tau T_c)]^{-1}}\kappa_0. \tag{46}$$

This expression enables us to eliminate κ_0 in favor of $\kappa_{\rm GL}$.

The case with p-wave impurity scattering may be treated similarly by using Eqs. (B8) and (B9) for $\tilde{f}_N^{(1)}$ and $J_N^{(3)}$, respectively. The resulting $\kappa_{\rm GL}$ is given by Eq. (46) with a replacement of τ by the transport lifetime $\tau_{\rm tr}$ defined through

$$\frac{1}{\tau_{\rm tr}}\equiv\frac{1}{\tau}-\frac{1}{\tau_1}, \tag{47}$$

in agreement with Eilenberger.[12]

H. Eilenberger's results

I now clarify the connection with Eilenberger's well-known results.[12] They are obtained by extracting from $I^{(4)}_{N_1N_2N_3N_4}$ of Eq. (20a) a part which may be expressed in terms of $\beta_{\rm A}=1.16$ of Eq. (21).

To see this, let us start from an alternative expression of $I^{(4)}_{N_1N_2N_3N_4}$ for $N_1+N_2=N_3+N_4$:

$$I^{(4)}_{N_1N_2N_3N_4}=\sum_{N_a}\frac{V}{2}\sum_{\alpha=1}^{2}|\psi_{N_a\mathbf{0}\alpha}(\mathbf{0})|^2\langle N_1N_2|N_1+N_2-N_aN_a\rangle \times\langle N_3N_4|N_1+N_2-N_aN_a\rangle. \tag{48}$$

Here $\psi_{N_a\mathbf{0}\alpha}(\mathbf{0})$ and $\langle N_1N_2|N_3N_4\rangle$ are the quasiparticle wave function and the overlap integral defined by Eqs. (3.12) and (3.23) of Ref. 28, respectively. This identity can be proved by using Eqs. (3.22) and (3.24) of Ref. 28 and noting $\psi^{(c)}_{N\mathbf{q}}(\mathbf{r})=\psi^{(r)}_{N\mathbf{q}}(2\mathbf{r})$ which both denote the present $\psi_{N\mathbf{q}}(\mathbf{r})$. If we retain only terms of $N_a=0$ in Eq. (48) and use $(V/2)\Sigma_{\alpha=1}^2|\psi_{0\mathbf{0}\alpha}(\mathbf{0})|^2=\beta_{\rm A}$, we obtain an approximate expression for Eq. (48) as

$$\begin{aligned}I^{(4)}_{N_1N_2N_3N_4}&\approx\beta_{\rm A}\langle N_1N_2|N_1+N_20\rangle\langle N_3N_4|N_1+N_20\rangle\\&=\frac{(N_1+N_2)!}{2^{N_1+N_2}\sqrt{N_1!N_2!N_3!N_4!}}\beta_{\rm A}\\&\equiv I^{(4\rm E)}_{N_1N_2N_3N_4}.\end{aligned} \tag{49}$$

Now Eilenberger's approximation for κ_2 is given by Eqs. (2.7), (2.8), and (6.5) of his paper[12] and corresponds to

$$\kappa_2\approx(\kappa_0^2S_4^{(\rm E)}/2S_2^2\beta_{\rm A})^{1/2}\equiv\kappa_2^{(\rm E)}, \tag{50}$$

in Eq. (34b), where $S_4^{(\rm E)}$ is obtained from Eq. (35b) by replacing $I^{(4)}$ by $I^{(4\rm E)}$. Indeed, this procedure yields numerical agreements with his results. As seen below in Sec. III B, however, this approximation is not correct quantitatively far beyond his estimation $\sim 1\%$.

It should also be noted that Eilenberger's definition of κ_2 by Eq. (50) is different from Maki's through Eq. (34b) with respect to

$$\eta\equiv S_A/S_2^2\beta_{\rm A}. \tag{51}$$

I resume Maki's definition through Eq. (34b) where κ_2 has a one-to-one correspondence with the initial slope of the magnetization. This is certainly more preferable than expressing the slope with two parameters $\kappa_2^{(\rm E)}$ and η.

I finally comment on Eilenberger's analytic expression for η. In addition to approximation (49), it was obtained by integrating the Maxwell equation with a removal of a common operator; see the argument above Eq. (6.4).[12] However, this procedure may bring an erroneous constant. Indeed, his $B_0(\mathbf{r})$ of Eq. (6.4) does not satisfy the required condition $\int B_0(\mathbf{r})d\mathbf{r}=0$. Thus, his expression for η is incorrect in the two respects and cannot be obtained by adopting approximation (49) in Eq. (51).

III. NUMERICAL RESULTS

A. Numerical procedures

I have adopted the same parameters as those of Eilenberger:[12]

$$\xi_{\rm E}/l_{\rm tr}\equiv 1/2\pi T_c\tau_{\rm tr},\quad l_{\rm tr}/l\equiv\tau_{\rm tr}/\tau, \tag{52}$$

to express different impurity concentrations. Numerical calculations of Eqs. (33)–(35) have been performed for each set of parameters by restricting every summation over the Matsubara frequencies for those satisfying $\varepsilon_n\leqslant\varepsilon_c$. Choosing $\varepsilon_c=50$–100 has been sufficient to obtain an accuracy of $\sim 0.01\%$ for κ_2. On the other hand, summations over the Landau levels have been truncated at $N=N_{\rm cut}$ where I put $\mathcal{R}_{N_{\rm cut}}=1$ in the calculation of $K_N^{N'}$; see Sec. II F for the details. Enough convergence has been obtained by choosing $N_{\rm cut}=4$, 40, 100, 200, 500, and 2000 for $\xi_{\rm E}/l_{\rm tr}=50$, 1.0, 0.5, 0.1, and 0.05, respectively. Finally, integrations over θ have been performed by Simpson's formula with $N_{\rm cut}+1$ integration points for $0\leqslant\theta\leqslant\pi/2$.

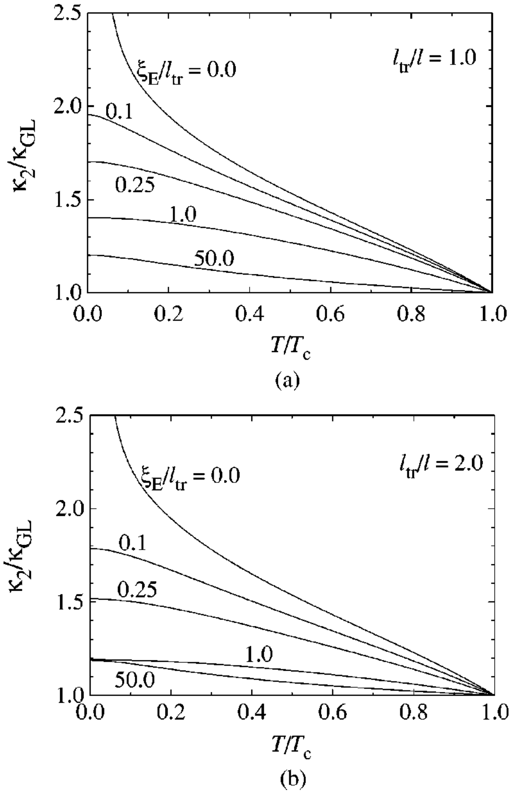

FIG. 1. Temperature dependence of κ_2/κ_{GL} for several values of ξ_E/l_{tr} in the extreme type-II case $\kappa_{GL}=50$. (a) $l_{tr}/l=1.0$; (b) $l_{tr}/l=2.0$.

B. Results for κ_2

Figure 1 shows κ_2/κ_{GL} as a function of T/T_c for different impurity concentrations. The upper one is for $l_{tr}/l=1.0$, i.e., the case without *p*-wave impurity scattering, whereas the lower one is for $l_{tr}/l=2.0$. They are calculated in an extreme type-II case of $\kappa_{GL}=50$, so that they directly correspond to Eilenberger's results for $l_{tr}/l=1$ and 2, respectively.[12] These curves show qualitatively the same behaviors as those of Eilenberger's, including the divergence in the clean limit for $T\to 0$, as predicted by Maki and Tsuzuki.[8] Except the curves in the dirty limit, however, marked quantitative differences are seen. For example, $\kappa_2(T=0)/\kappa_{GL}$ for $(\xi_E/l_{tr},l_{tr}/l)=(1.0,1.0)$ is 1.40 from the present calculation, whereas it is 1.50 from Eilenberger's. Thus, we realize that Eilenberger's approximation (50) yields quantitative errors of $\lesssim 20\%$ for the deviation $\kappa_2/\kappa_{GL}-1$. Comparing the two figures, we observe the following: (i) The results in the dirty limit are the same between $l_{tr}/l=1$ and 2; (ii) *p*-wave scattering has a general tendency to lower the values of κ_2, and also produces a nonmonotonic behavior in κ_2/κ_{GL} as a function of ξ_E/l_{tr}.

Figure 2 displays η defined by Eq. (51) as a function of T/T_c for $\xi_E/l_{tr}=0.05$-50.0 and $l_{tr}/l=1.0$. This quantity becomes relevant for small values of κ_{GL} at low temperatures, as may be realized by Eq. (34b). The curves also deviate substantially from Eilenberger's results. For example, η for $\xi_E/l_{tr}=0.25$ at $T=0$ is 1.34 from the present calculation, whereas it is ~ 1.11 from Eilenberger's. Generally, the values are larger than those of Eilenberger's. This fact implies that $\kappa_2(T)$ for $\kappa_{GL}\sim 1$ becomes smaller than the evaluation of Eilenberger.

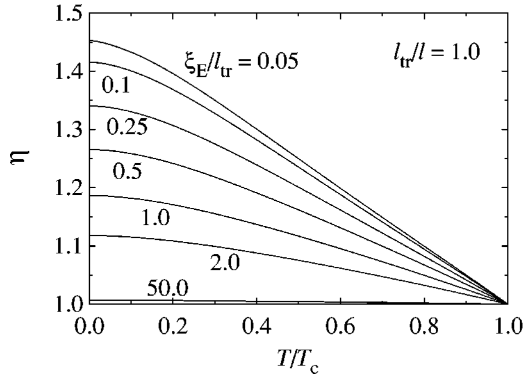

FIG. 2. Temperature dependence of η defined by Eq. (51) for several values of ξ_E/l_{tr} with $l_{tr}/l=1.0$.

To see the dependence of κ_2/κ_{GL} on κ_{GL} explicitly, I have performed a calculation of κ_2 near the type-I–type-II boundary of $\kappa_{GL}=1.0$. Figure 3 plots the results for $\xi_E/l_{tr}=0.0$–50.0 and $l_{tr}/l=1$. Compared with Fig. 1(a), we observe that each curve is slightly shifted downward. However, the changes are surprisingly small, considering the closeness to the type-I–type-II boundary. We thus realize that the factor $S_A/S_2^2=\eta\beta_A$ in Eq. (34b) can be neglected practically for $\kappa_{GL}\gtrsim 5$, as already observed by Eilenberger.[12]

The above calculations are performed for an idealized spherical Fermi surface. However, real superconductors are often characterized by complicated Fermi surfaces. To see the dependence of κ_2/κ_{GL} on Fermi-surface structures, I have performed an isotropic two-dimensional calculation described in Sec. II C. Figure 4 shows the results, where the parameters are the same as those in Fig. 1. The curves for $\xi_E/l_{tr}=50$ are almost the same as those in Fig. 1. Thus, in the dirty limit, we have a universal curve which depends neither on detailed Fermi-surface structures nor fine features of the impurity scattering. As the system becomes cleaner, however, differences due to the two factors emerge eventually. In fact, we observe that each curve for $\xi_E/l_{tr}\lesssim 1.0$ in Fig. 4 deviates far less from 1 than the corresponding one in Fig. 1, and the temperature dependence is also weaker. An-

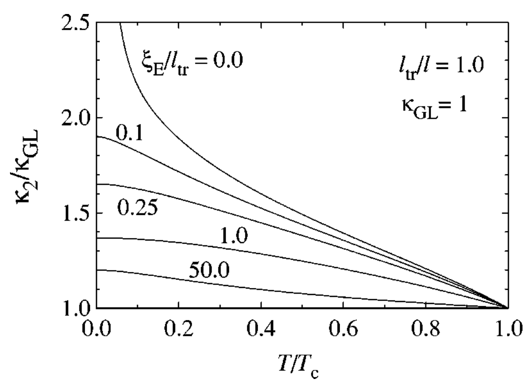

FIG. 3. Temperature dependence of κ_2/κ_{GL} for $\kappa_{GL}=1$ with $l_{tr}/l=1.0$.

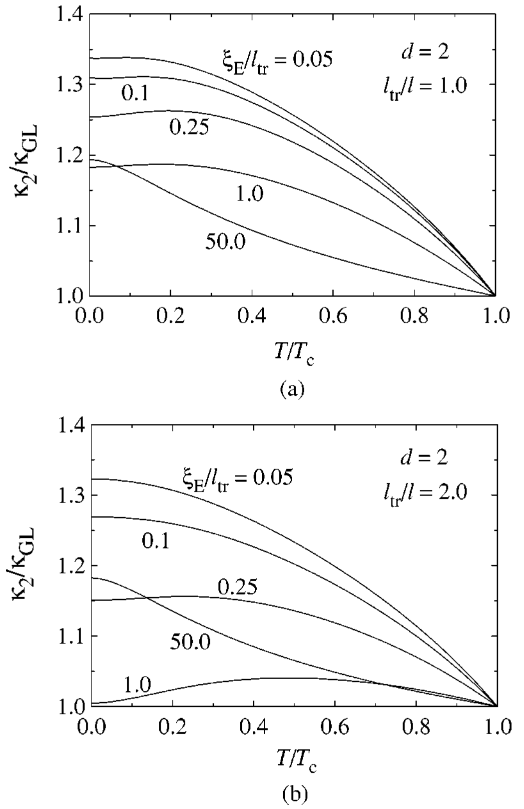

FIG. 4. Temperature dependence of $\kappa_2/\kappa_{\rm GL}$ for an isotropic two-dimensional system in the extreme type-II case $\kappa_{\rm GL}=50$. (a) $l_{\rm tr}/l=1.0$; (b) $l_{\rm tr}/l=2.0$.

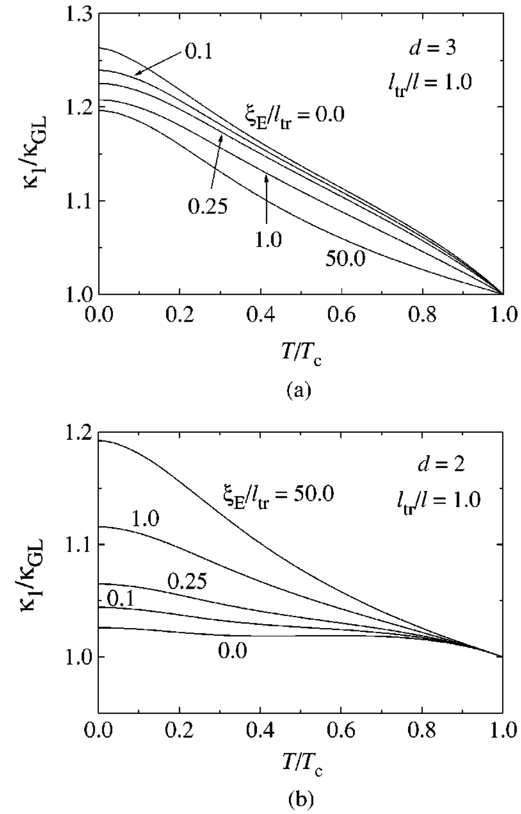

FIG. 5. Temperature dependence of $\kappa_1/\kappa_{\rm GL}$ for several values of $\xi_{\rm E}/l_{\rm tr}$ with $l_{\rm tr}/l=1.0$. (a) $d=3$; (b) $d=2$.

other point to be mentioned is that, even for $\xi_{\rm E}/l_{\rm tr}=0.05$, we see no trace of divergence as $T\rightarrow 0$. Indeed, a closer examination of the analytic results by Maki and Tsuzuki[8] and Eilenberger[12] enables us to realize that it is the region $\theta\sim 0$ in three dimensions which is responsible for the divergence of κ_2. Thus, we may conclude that κ_2 in two dimensions remains finite even in the clean limit as $T\rightarrow 0$. In general, κ_2 will remain finite if the relevant Fermi surface does not close along the direction of the magnetic field.

C. Results for κ_1

The Maki parameter κ_1 is defined by[2]

$$\kappa_1\equiv H_{c2}/\sqrt{2}H_c, \tag{53}$$

where $H_c=H_c(T)$ is the thermodynamic critical field. The preceding results for κ_2 suggest that $\kappa_1(T)/\kappa_{\rm GL}$ may also exhibit considerable dependence on detailed Fermi-surface structures.

Figure 5 compares $\kappa_1(T)/\kappa_{\rm GL}$ between two and three dimensions for $l_{\rm tr}/l=1.0$. The curves for $\xi_{\rm E}/l_{\rm tr}=50$ show almost the same behavior. As $\xi_{\rm E}/l_{\rm tr}$ becomes smaller, however, the two cases display a marked difference. Indeed, $\kappa_1(T)/\kappa_{\rm GL}$ is seen to increase (decrease) in three (two) dimensions as $\xi_{\rm E}/l_{\rm tr}\rightarrow 0$.

Figure 6 shows curves of $\kappa_1(T)/\kappa_{\rm GL}$ in two and three dimensions for $l_{\rm tr}/l=2.0$. Again the p-wave impurity scattering is seen to lower the value of $\kappa_1/\kappa_{\rm GL}$, and also introduces nonmonotonicity in $\kappa_1/\kappa_{\rm GL}$ as a function of $\xi_{\rm E}/l_{\rm tr}$. Especially in two dimensions for $\xi_{\rm E}/l_{\rm tr}=0.1$–$1.0$, $\kappa_1/\kappa_{\rm GL}$ becomes smaller than 1 over finite temperature ranges, i.e., the empirical inequality $\kappa_2\geqslant\kappa_1\geqslant\kappa_{\rm GL}$ is not satisfied here, even without spin paramagnetism.[11]

A substantial dependence of H_{c2} on Fermi-surface structures may be realized more clearly by looking at the temperature dependence of the reduced critical field introduced by Helfand and Werthamer:[5]

$$h^*(t)\equiv\frac{H_{c2}(t)}{-dH_{c2}(t)/dt\big|_{t=1}}, \tag{54}$$

where $t\equiv T/T_c$. Figure 7 compares $h^*(t)$ between two and three dimensions for both the clean and dirty limits. The curves coincide in the dirty limit, whereas those in the clean limit show a marked quantitative difference. We also observe that $h^*(t)$ in two dimensions is a rather sensitive function of purity. A considerable reduction of $h^*_{d=2}(t)$ in the pure limit from $h^*_{d=3}(t)$ may be attributed to the pair breaking by supercurrent. This effect is more effective in two dimensions. Indeed, a point on the cylindrical Fermi surface is equivalent to a point on the equator of the spherical Fermi surface perpendicular to **H** where the pair breaking is most effective. This fact can be seen clearly in the polar-angle dependence of the density of states calculated by Brandt, Pesch, and Tewordt.[29] Put it another way, if the relevant Fermi surface does not have a closed orbit perpendicular to **H**, the corre-

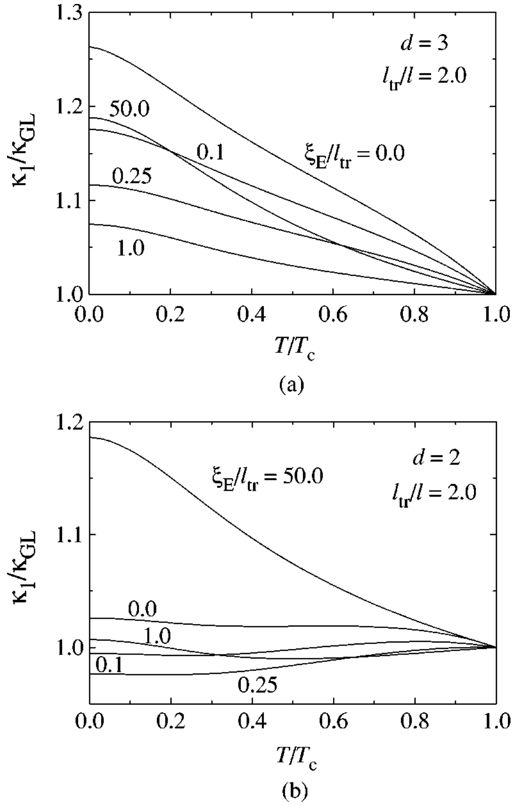

FIG. 6. Temperature dependence of κ_1/κ_{GL} for several values of ξ_E/l_{tr} with $l_{tr}/l=2.0$. (a) $d=3$; (b) $d=2$.

sponding $h^*(t)$ in the clean limit will be enhanced over the prediction for the spherical Fermi surface.

A considerable reduction of $h^*(t)$ or $\kappa_1(t)$ in the presence of spin paramagnetism was established by Werthamer, Helfand, and Hohenberg,[6] and also by Maki.[11] The present results indicate unambiguously that the Fermi-surface structure is also an important factor for $h^*(t)$ in clean systems, as already noticed by Helfand and Werthamer,[5] Hohenberg and Werthamer,[30] and Werthamer and McMillan.[31]

D. Results for the pair potential

A quantity of fundamental importance is the coefficient Δ_0, which is equal to the spatial average $\sqrt{\langle|\Delta(\mathbf{r})|^2\rangle}$ of the

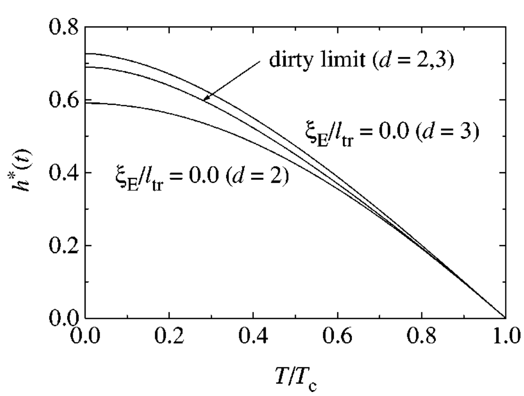

FIG. 7. Temperature dependence of the reduced critical field $h^*(t)$ for the dirty limit of $d=2,3$ (mid curve) and the clean limit of $d=2$ (lower curve) and $d=3$ (upper curve).

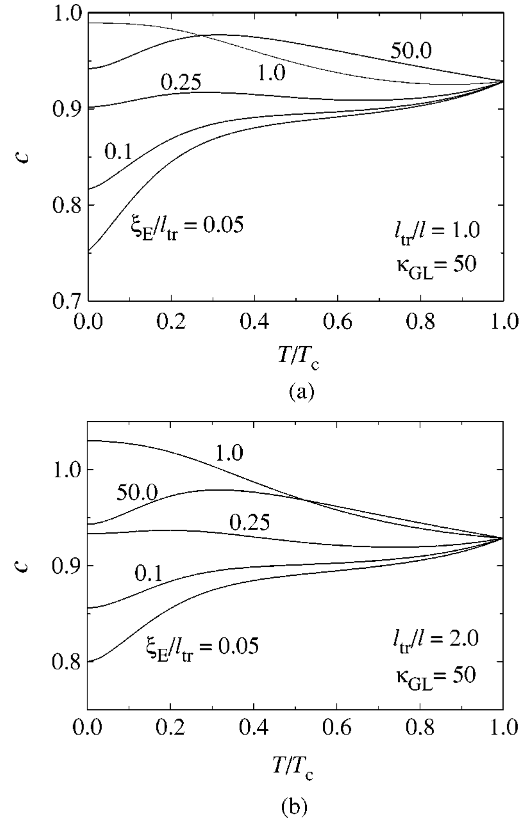

FIG. 8. The coefficient $c(T)\equiv(1-B/H_{c2})^{1/2}\Delta(T)/\Delta_0(B,T)$ in the extreme type-II case $\kappa_{GL}=50$ as a function of T/T_c for several values of ξ_E/l_{tr}. (a) $l_{tr}/l=1.0$; (b) $l_{tr}/l=2.0$.

pair potential and relevant to all thermodynamic and transport properties near H_{c2}. It is physically more meaningful to express it as a function of the real average field B in the bulk instead of H. Equation (36) shows that $\Delta_0(B)$ is proportional to $(H_{c2}-B)^{1/2}$ near H_{c2}. I here express this Δ_0 by using the energy gap $\Delta(T)$ at $B=0$ as

$$\Delta_0(B,T)=c(T)(1-B/H_{c2})^{1/2}\Delta(T). \tag{55}$$

Then the coefficient $c(T)$ should be of the order of 1.

Figure 8 calculated for the spherical Fermi surface displays temperature dependence of $c(T)$ in an extreme type-II case of $\kappa_{GL}=50$ for (a) $l_{tr}/l=1.0$ and (b) $l_{tr}/l=2.0$. Thus $c(T)\sim 1$, as expected, having the same value 0.929 at T_c. Differences among different ξ_E/l_{tr} grow at lower temperatures, and $c(T)$ for $\xi_E/l_{tr}\lesssim 0.1$ drops rapidly near $T=0$. Indeed, $c(T)$ in the clean limit for three dimensions is expected to reach 0 as $T\to 0$, corresponding to the divergence of κ_2. This also implies that the expansion in $\Delta(\mathbf{r})$ near H_{c2} is no longer valid in this limit.[14] The curves in the dirty limit are the same between $l_{tr}/l=1.0$ and $l_{tr}/l=2.0$. For $\xi_E/l_{tr}\lesssim 1.0$, however, each curve for $l_{tr}/l=2.0$ at low temperatures has larger values than the corresponding one for $l_{tr}/l=1.0$. Thus, finite p-wave scattering in clean systems tends to increase $c(T)$.

The coefficient $c(T)$ also increases mildly as κ_{GL} becomes smaller, as realized by comparing Fig. 9 for $\kappa_{GL}=1$ with Fig. 8(a) for $\kappa_{GL}=50$.

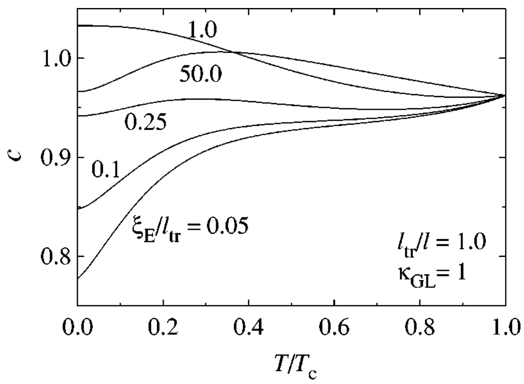

FIG. 9. The coefficient $c(T)$ for $\kappa_{GL}=1$ as a function of T/T_c for several values of ξ_E/l_{tr} with $l_{tr}/l=1.0$.

Figure 10 plots results of the two-dimensional calculations performed with the same parameters as those in Fig. 8. The curves for the dirty limit are the same between two and three dimensions. As the system becomes cleaner, however, the coefficient $c(T)$ for two dimensions becomes larger than the corresponding one for three dimensions. Thus, for clean systems, we observe once again a considerable dependence of the coefficient $c(T)$ on Fermi-surface structures.

IV. SUMMARY

This paper has presented revised calculations of the Maki parameters κ_1 and κ_2 as well as the spatial average $\langle|\Delta(\mathbf{r})|^2\rangle$ near H_{c2}. Eilenberger's results for κ_2 have been corrected appropriately, as described in Sec. II H. The analytic expressions derived in Secs. II E and II F have been useful to carry out efficient calculations for both two and three dimensions with isotropic Fermi surfaces and arbitrary impurity concentrations. Thereby found are large quantitative differences of the parameters between two and three dimensions (except in the dirty limit where there are no differences between the two cases). For example, no trace of divergence in $\kappa_2(T\to 0)$ is found for the clean limit in two dimensions.

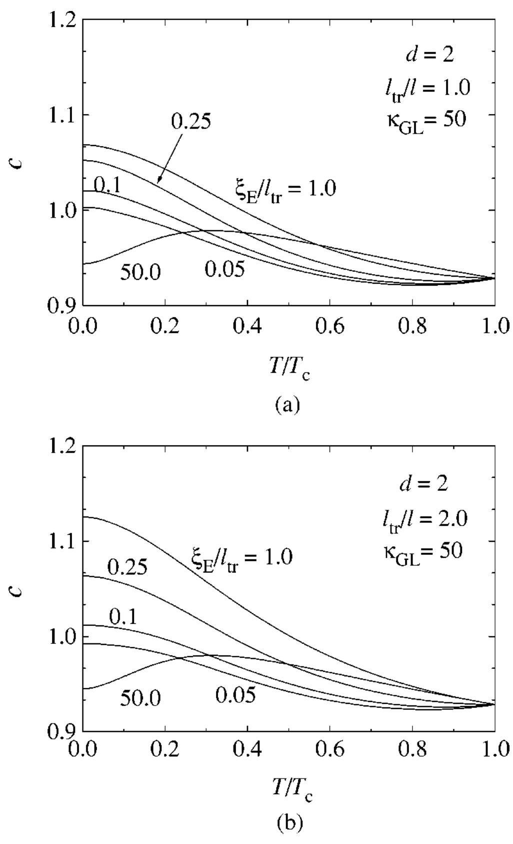

FIG. 10. The coefficient $c(T)$ in two dimensions with $\kappa_{GL}=50$ as a function of T/T_c for several values of ξ_E/l_{tr}. (a) $l_{tr}/l=1.0$; (b) $l_{tr}/l=2.0$.

The present results clearly indicate the necessity of considering detailed Fermi-surface structures from first-principles calculations for a quantitative understanding of the Maki parameters in clean superconductors. This was already recognized by Helfand and Werthamer,[5] by Hohenberg and Werthamer,[30] and also by Werthamer and McMillan[31] when their strong-coupling calculation could not explain a large deviation of κ_1/κ_{GL} observed in pure niobium[32,33] and vanadium[34] from the theoretical prediction of Helfand and Werthamer.[5] Efforts have been made along this line to establish a realistic calculation of κ_1, or equivalently, H_{c2}.[30,35–44] However, little progress seems to have been achieved with respect to κ_2.

The method developed here for κ_1 and κ_2 may be extended easily to include Fermi-surface structures and anisotropic pairings. Some of the necessary modifications are (i) to use the general expansion (13a) with even N for the pair potential, rather than Eq. (15); (ii) to use more convenient basis functions than $e^{im\varphi}$ in Eq. (13b) for describing the $\mathbf{k}_F$ dependence of $f(\varepsilon_n,\mathbf{k}_F,\mathbf{r})$, such as the Fermi-surface harmonics of Allen.[45–48] The corresponding matrix $\tilde{\mathcal{M}}$ in Eqs. (17a) and (17b) is no longer tridiagonal, but may be inverted rather easily with present high-speed computers.

ACKNOWLEDGMENTS

I am grateful to M. Endres and D. Rainer for discussions about free-energy functionals of the quasiclassical theory. This research was supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science, and Technology of Japan.

APPENDIX A: DERIVATION OF EQ. (4)

To obtain Eq. (4), let us start from Eilenberger's free-energy functional[15] per unit volume with B chosen as an independent variable instead of H. It is given in units of $N(0)\Delta(0)^2$ as

$$\frac{F(B)}{V}=\frac{1}{V}\int d\mathbf{r}\Bigg\{\frac{\kappa_0^2}{2}[B^2+(\boldsymbol{\nabla}\times\tilde{\mathbf{A}})^2]+|\Delta(\mathbf{r})|^2\ln\frac{T}{T_c}+2\pi T\sum_{n=0}^{\infty}\left[\frac{|\Delta(\mathbf{r})|^2}{\varepsilon_n}-\langle I(\varepsilon_n,\mathbf{k}_F,\mathbf{r})\rangle\right]\Bigg\}, \quad \text{(A1)}$$

where I is defined by

$$I\equiv\Delta^* f+\Delta f^\dagger+2\varepsilon_n(g-1)+\frac{f\langle f^\dagger\rangle+\langle f\rangle f^\dagger}{4\tau}+\frac{g\langle g\rangle-1}{2\tau}+(g-1)\hat{\mathbf{v}}\cdot\frac{f^\dagger(\boldsymbol{\nabla}-i\mathbf{A})f-f(\boldsymbol{\nabla}+i\mathbf{A})f^\dagger}{2ff^\dagger}. \tag{A2}$$

The functional derivatives of Eq. (A1) with respect to $f^\dagger$, Δ, and $\mathbf{A}$ lead to Eqs. (2a)–(2c), respectively. The last term in Eq. (A2) is slightly different from the original functional of Eilenberger where $g\hat{\mathbf{v}}$ appears in place of $(g-1)\hat{\mathbf{v}}$.[15] Although it does not change Eq. (2) at all, it is found numerically that the modification is necessary for F to have its absolute minimum with respect to Δ, $\mathbf{A}$, and $f=f(\Delta,\mathbf{A})$ satisfying Eq. (2a), as anticipated by Eilenberger.[15] It should be noted that Pesch and Kramer[49] also adopted Eq. (A1) as a basis for their numerical calculations. More recently, Endres and Rainer[50] performed a numerical calculation of the free energy for both an SN contact and a single vortex based on Eq. (A1), and compared the results with those from three free-energy functionals obtained from the Luttinger-Ward functional. They found numerical agreements among the values from four different expressions.

Following Doria, Gubernatis, and Rainer,[25] I now rewrite the right-hand side of Eq. (A1) in terms of

$$\mathbf{r}'\equiv\mathbf{r}/\lambda,\quad B_\lambda\equiv\lambda^2 B,\quad \tilde{\mathbf{A}}_\lambda(\mathbf{r}')\equiv\lambda\tilde{\mathbf{A}}(\lambda\mathbf{r}'),$$
$$\Delta_\lambda(\mathbf{r}')\equiv\Delta(\lambda\mathbf{r}'),\quad f_\lambda(\varepsilon_n,\mathbf{k}_{\rm F},\mathbf{r}')\equiv f(\varepsilon_n,\mathbf{k}_{\rm F},\lambda\mathbf{r}'). \tag{A3}$$

I then differentiate the resulting expression with respect to λ and put $\lambda=1$. Since procedure (A3) does not change the value of F/V, we have $(\partial/\partial\lambda)(F/V)|_{\lambda=1}=0$ from the left-hand side. As for the right-hand side, the only implicit dependence to be considered is the one from B_λ; those from f_λ, Δ_λ, and $\tilde{\mathbf{A}}_\lambda$ can be neglected due to the stationarity of Eq. (2). We thereby obtain

$$0=\frac{\partial(F/V)}{\partial B_\lambda}\frac{\partial B_\lambda}{\partial\lambda}\bigg|_{\lambda=1}-2\kappa_0^2B^2-\frac{2\kappa_0^2}{V}\int d\mathbf{r}\,(\boldsymbol{\nabla}\times\tilde{\mathbf{A}})^2-\frac{\pi T}{V}\sum_{n=0}^{\infty}\int d\mathbf{r}\left\langle\frac{f^\dagger\hat{\mathbf{v}}\cdot(\boldsymbol{\nabla}-i\mathbf{A})f-f\hat{\mathbf{v}}\cdot(\boldsymbol{\nabla}+i\mathbf{A})f^\dagger}{1+g}\right\rangle. \tag{A4}$$

Using the thermodynamic relation $\partial(F/V)/\partial B_\lambda|_{\lambda=1}=\kappa_0^2H$ in the present units, we arrive at Eq. (4).

APPENDIX B: EXTENSION TO THE CASE WITH p-WAVE IMPURITY SCATTERING

In the presence of p-wave impurity scattering, Eq. (2a) is replaced by

$$\left[\varepsilon_n+\frac{\langle g\rangle}{2\tau}+\frac{d\hat{\mathbf{k}}\cdot\langle\hat{\mathbf{k}}'g\rangle}{2\tau_1}+\frac{\hat{\mathbf{v}}}{2}\cdot(\boldsymbol{\nabla}-i\mathbf{A})\right]f=\left(\Delta+\frac{\langle f\rangle}{2\tau}+\frac{d\,\hat{\mathbf{k}}\cdot\langle\hat{\mathbf{k}}'f\rangle}{2\tau_1}\right)g, \tag{B1}$$

where $\langle\hat{\mathbf{k}}'g\rangle\equiv\langle\hat{\mathbf{k}}'g(\varepsilon_n,\mathbf{k}_{\rm F}',\mathbf{r})\rangle$, for example, and $d=2,3$ is the dimension of the system. This brings additional terms on the right-hand side of Eqs. (17a) and (17b) as

$$\sum_{N'}\tilde{\mathcal{M}}_{NN'}\tilde{f}_{N'}^{(1)}=\delta_{N0}\left(1+\frac{\langle\tilde{f}_0^{(1)}\rangle}{2\tau}+\frac{d\cos\theta\langle\tilde{f}_0^{(1)}\cos\theta'\rangle}{2\tau_1}\right)+\delta_{N1}\frac{d\sin\theta\langle\tilde{f}_1^{(1)}\sin\theta'\rangle}{4\tau_1} \tag{B2}$$

$$\sum_{N'}\tilde{\mathcal{M}}_{NN'}\tilde{f}_{N'}^{(3)}=\delta_{N0}\left(\frac{\langle\tilde{f}_0^{(3)}\rangle}{2\tau}+\frac{d\cos\theta\langle\tilde{f}_0^{(3)}\cos\theta'\rangle}{2\tau_1}\right)+\delta_{N1}\frac{d\sin\theta\langle\tilde{f}_1^{(3)}\sin\theta'\rangle}{4\tau_1}+J_N^{(3)}+J_N^{(A)}, \tag{B3}$$

where $J_N^{(A)}$ is given by Eq. (19c), and $J_N^{(3)}$ is defined instead of Eq. (19b) by

$$\begin{aligned}J_N^{(3)}\equiv&-\frac{1}{2}\sum_{N'}(-1)^{N'}I^{(4)}_{NN'N+N'0}\tilde{f}^{(1)}_{N'}\tilde{f}^{(1)}_{N+N'}\left(1+\frac{\langle\tilde{f}_0^{(1)}\rangle}{2\tau}+\frac{d\cos\theta\langle\tilde{f}_0^{(1)}\cos\theta'\rangle}{2\tau_1}\right)\\&+\frac{1}{4}\sum_{N'}(-1)^{N'}I^{(4)}_{NN'N'N}\left(\frac{\langle\tilde{f}^{(1)}_{N'}\tilde{f}^{(1)}_{N'}\rangle}{\tau}+\frac{d\cos\theta\langle\tilde{f}^{(1)}_{N'}\tilde{f}^{(1)}_{N'}\cos\theta'\rangle}{\tau_1}\right)\tilde{f}^{(1)}_N\\&+\frac{d\sin\theta}{8\tau_1}\sum_{N'}(-1)^{N'}[-I^{(4)}_{NN'N+N'-11}\tilde{f}^{(1)}_{N'}\tilde{f}^{(1)}_{N+N'-1}\langle\tilde{f}^{(1)}_1\sin\theta'\rangle\\&+I^{(4)}_{NN'N'-1N+1}\langle\tilde{f}^{(1)}_{N'}\tilde{f}^{(1)}_{N'-1}\sin\theta'\rangle\tilde{f}^{(1)}_{N+1}+I^{(4)}_{NN'N'+1N-1}\langle\tilde{f}^{(1)}_{N'}\tilde{f}^{(1)}_{N'+1}\sin\theta'\rangle\tilde{f}^{(1)}_{N-1}].\end{aligned} \tag{B4}$$

Equation (B2) can be solved in the same way as Eq. (26) to yield

$$\tilde{f}_N^{(1)} = \tilde{K}_N^0 \left(1 + \frac{\langle \tilde{f}_0^{(1)} \rangle}{2\tau} + \frac{d \cos\theta \langle \tilde{f}_0^{(1)} \cos\theta' \rangle}{2\tau_1} \right) + \tilde{K}_N^1 \frac{d \sin\theta \langle \tilde{f}_1^{(1)} \sin\theta' \rangle}{4\tau_1}. \tag{B5}$$

From Eq. (B5), we obtain self-consistent equations for $\langle \tilde{f}_0^{(1)} \rangle$, $\langle \tilde{f}_0^{(1)} \cos\theta \rangle$, and $\langle \tilde{f}_1^{(1)} \sin\theta \rangle$ as

$$\mathcal{K} \begin{bmatrix} \langle \tilde{f}_0^{(1)} \rangle \\ \langle \tilde{f}_0^{(1)} \cos\theta \rangle \\ \langle \tilde{f}_1^{(1)} \sin\theta \rangle \end{bmatrix} = \begin{bmatrix} \langle \tilde{K}_0^0 \rangle \\ \langle \tilde{K}_0^0 \cos\theta \rangle \\ \langle \tilde{K}_1^0 \sin\theta \rangle \end{bmatrix}, \tag{B6}$$

where the matrix $\mathcal{K}$ is defined by

$$\mathcal{K} \equiv \begin{bmatrix} 1 - \dfrac{\langle \tilde{K}_0^0 \rangle}{2\tau} & -\dfrac{d \langle \tilde{K}_0^0 \cos\theta \rangle}{2\tau_1} & \dfrac{d \langle \tilde{K}_1^0 \sin\theta \rangle}{4\tau_1} \\ -\dfrac{\langle \tilde{K}_0^0 \cos\theta \rangle}{2\tau} & 1 - \dfrac{d \langle \tilde{K}_0^0 \cos^2\theta \rangle}{2\tau_1} & \dfrac{d \langle \tilde{K}_1^0 \sin 2\theta \rangle}{8\tau_1} \\ -\dfrac{\langle \tilde{K}_1^0 \sin\theta \rangle}{2\tau} & -\dfrac{d \langle \tilde{K}_1^0 \sin 2\theta \rangle}{4\tau_1} & 1 - \dfrac{d \langle \tilde{K}_1^1 \sin^2\theta \rangle}{4\tau_1} \end{bmatrix}. \tag{B7}$$

Noting $K_{N'}^N = K_{N'}^N(\tilde{\varepsilon}_n, \beta)$ as seen from Eqs. (41)–(43) with β defined in Eq. (9), we immediately realize that $\langle \tilde{K}_0^0 \cos\theta \rangle = 0$ in Eq. (B6) and $\mathcal{K}_{2j} = \mathcal{K}_{j2} = 0$ for $j = 1,3$ in Eq. (B7). Thus, Eq. (B6) can be solved easily with $\langle \tilde{f}_0^{(1)} \cos\theta \rangle = 0$. Substituting the resulting expressions of $\langle \tilde{f}_0^{(1)} \rangle$ and $\langle \tilde{f}_1^{(1)} \sin\theta \rangle$ into Eq. (B5), we obtain

$$\tilde{f}_N^{(1)} = \frac{\left(1 - \dfrac{d}{4\tau_1} \langle \tilde{K}_1^1 \sin^2\theta' \rangle \right) \tilde{K}_N^0 + \dfrac{d}{4\tau_1} \langle \tilde{K}_1^0 \sin\theta' \rangle \tilde{K}_N^1 \sin\theta}{\left(1 - \dfrac{1}{2\tau} \langle \tilde{K}_0^0 \rangle \right) \left(1 - \dfrac{d}{4\tau_1} \langle \tilde{K}_1^1 \sin^2\theta' \rangle \right) + \dfrac{d}{8\tau\tau_1} \langle \tilde{K}_1^0 \sin\theta' \rangle^2}. \tag{B8}$$

Equation (B4) is also simplified into

$$\begin{aligned} J_N^{(3)} \equiv & -\frac{1}{2} \sum_{N'} (-1)^{N'} I^{(4)}_{NN'N+N'0} \tilde{f}_{N'}^{(1)} \tilde{f}_{N+N'}^{(1)} \left(1 + \frac{\langle \tilde{f}_0^{(1)} \rangle}{2\tau} \right) + \frac{1}{4\tau} \sum_{N'} (-1)^{N'} I^{(4)}_{NN'N'N} \langle \tilde{f}_{N'}^{(1)} \tilde{f}_{N'}^{(1)} \rangle \tilde{f}_N^{(1)} \\ & + \frac{d \sin\theta}{8\tau_1} \sum_{N'} (-1)^{N'} [-I^{(4)}_{NN'N+N'-11} \tilde{f}_{N'}^{(1)} \tilde{f}_{N+N'-1}^{(1)} \langle \tilde{f}_1^{(1)} \sin\theta' \rangle + I^{(4)}_{NN'N'-1N+1} \langle \tilde{f}_{N'}^{(1)} \tilde{f}_{N'-1}^{(1)} \sin\theta' \rangle \tilde{f}_{N+1}^{(1)} \\ & + I^{(4)}_{NN'N'+1N-1} \langle \tilde{f}_{N'}^{(1)} \tilde{f}_{N'+1}^{(1)} \sin\theta' \rangle \tilde{f}_{N-1}^{(1)}]. \end{aligned} \tag{B9}$$

Equation (B3) can be treated similarly to obtain $\langle \tilde{f}_0^{(3)} \rangle$ which appears in Eq. (17c). Then a straightforward calculation leads to the same expression (28) for $\langle \tilde{f}_0^{(3)} \rangle$ with $\tilde{f}_N^{(1)}$ and $J_N^{(3)}$ replaced by Eqs. (B8) and (B9), respectively. Another relevant quantity in Eq. (17c) is $\langle \tilde{f}_0^{(1)\prime} \rangle$, as seen from Eq. (30). Differentiating Eq. (B2) with respect to B and solving the resulting equation self-consistently, we also obtain Eq. (32) for $\langle \tilde{f}_0^{(1)\prime} \rangle$ with $\tilde{f}_N^{(1)}$ in Eq. (19a) replaced by Eqs. (B8).

It hence follows that Eqs. (34) and (35) remain the same in the presence of the p-wave impurity scattering with $\tilde{f}_N^{(1)}$ and $J_N^{(3)}$ replaced by Eqs. (B8) and (B9), respectively.

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