Magnetic-field and temperature dependence of the superconducting gap through current-density functional theory for superconductors

Katsuhiko Higuchi [1,*] Naoki Matsumoto,[1] Yuki Kamijo,[2] and Masahiko Higuchi [2]
[1]*Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8527, Japan*
[2]*Department of Physics, Faculty of Science, Shinshu University, Matsumoto 390-8621, Japan*

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Quantitative prediction of the gap behavior via first-principles calculations has thus far been restricted to temperature dependence. Here, we present a gap equation developed based on the current-density functional theory for superconductors. This equation is applicable to superconductors immersed in a magnetic field and enables us to quantitatively describe the magnetic-field and temperature dependence of the superconducting gap. We also develop a practical scheme in which the gap equation is solved simultaneously with a proposed relation between the energy gain of the superconducting state at zero magnetic field and that at a finite magnetic field. The presented scheme is applied to aluminum immersed in a magnetic field, and successfully reveals the temperature and magnetic-field dependences of the superconducting gap. The critical magnetic field thus obtained shows good agreement with experimental results.

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I. INTRODUCTION

First-principles calculation methods utilizing the density functional theory [1,2] (DFT) are widely employed for quantitative prediction of material properties. DFT-based theories for superconductors provide well-developed first-principles calculation methods [3–5]. Oliveira *et al.* first developed the DFT-based theory for superconductors [3]. Lüders *et al.* extended this theory by adding the density matrix of the nuclei to the members of basic variables, to treat electron-electron and electron-phonon interactions on the same footing [4,5]. This extended theory has been successfully applied to various systems [5–24].

DFT-based theories for superconductors [3–5] can predict the critical temperature (T_c) and temperature dependence of the order parameter of the superconducting state (OPSS). However, they cannot predict the critical magnetic field (B_c) or the magnetic-field dependence of the OPSS because they cannot consider superconductors immersed in a magnetic field. B_c is related to the critical current (Silsbee's rule [25,26]), which provides the upper limit of the current that can flow through the superconductor while maintaining the superconducting state. Therefore, the prediction of B_c as well as T_c is crucial for the application of superconductors to electrical power engineering devices, magnetic energy storage systems, and other systems.

To predict the critical magnetic field, DFT-based theories for superconductors should be extended so that they can treat superconductors immersed in a magnetic field. For this, the spin DFT for superconductors (SpinSCDFT) has been developed by Linscheid *et al.* [21] and is applied to a free electron gas featuring an exchange splitting, a phononic pairing field, and a Coulomb repulsion [22]. However, the effects of the currents are not taken into consideration in the SpinSCDFT [21,22]. To incorporate the effect of currents and to discuss the Meissner effect, we have developed a current-density functional theory (CDFT) for superconductors [27] based on the extended constrained-search theory [28–34]. This theory is regarded as an extension of the CDFT for the normal state [35–42] so that it can treat superconductors immersed in a magnetic field with considering the effects of the currents. In this paper, a gap equation is developed based on the CDFT for superconductors, considering the interaction between the magnetic field and electron spin (spin-Zeeman effect). This gap equation enables us to describe the gap behavior with respect to the magnetic field and temperature. In addition, a practical scheme to solve the gap equation is presented. We apply the practical scheme to aluminum immersed in a magnetic field. It is shown that the presented scheme successfully demonstrates the magnetic-field and temperature dependences of the superconducting gap and predicts the critical magnetic field for aluminum.

II. GAP EQUATION BASED ON THE CURRENT-DENSITY FUNCTIONAL THEORY FOR SUPERCONDUCTORS

A. Outline of the current-density functional theory for superconductors

We have developed the CDFT for superconductors [27] based on the extended constrained-search theory [28–34], in which the spin-Zeeman effect is not taken into consideration. In this subsection, we present the outline of the CDFT for superconductors with taking the spin-Zeeman effect into consideration.

*khiguchi@hiroshima-u.ac.jp

Let us consider the superconductor immersed in a magnetic field, the Hamiltonian of which is given by

$$\hat{H} = \hat{T} + \hat{W}_1 + \hat{W}_2 + e\int \boldsymbol{A}_{\rm given}(\boldsymbol{r})\cdot\hat{\boldsymbol{j}}_p^{(T)}(\boldsymbol{r})d^3r + e\int \boldsymbol{A}_{\rm given}(\boldsymbol{r})\cdot\hat{\boldsymbol{j}}_{M_s}(\boldsymbol{r})d^3r + \frac{e^2}{2m}\int \boldsymbol{A}_{\rm given}(\boldsymbol{r})^2\hat{n}(\boldsymbol{r})d^3r + \int v_{\rm ext}(\boldsymbol{r})\hat{n}(\boldsymbol{r})d^3rd\zeta, \tag{1}$$

with

$$\hat{T} = \int \psi^\dagger(\boldsymbol{r}\zeta)\frac{\boldsymbol{p}^2}{2m}\psi(\boldsymbol{r}\zeta)d^3rd\zeta, \tag{2}$$

$$\hat{W}_1 = \frac{e^2}{2}\iint \frac{\psi^\dagger(\boldsymbol{r}\zeta)\psi^\dagger(\boldsymbol{r}'\zeta')\psi(\boldsymbol{r}'\zeta')\psi(\boldsymbol{r}\zeta)}{|\boldsymbol{r}-\boldsymbol{r}'|}d^3rd\zeta d^3r'd\zeta', \tag{3}$$

$$\hat{W}_2 = \frac{1}{2}\iint \hat{\Delta}^\dagger(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)w(\boldsymbol{r}_1\zeta_1\boldsymbol{r}_2\zeta_2;\boldsymbol{r}_3\zeta_3\boldsymbol{r}_4\zeta_4) \times \hat{\Delta}(\boldsymbol{r}_4\zeta_4,\boldsymbol{r}_3\zeta_3)d^3r_1d\zeta_1d^3r_2d\zeta_2d^3r_3d\zeta_3d^3r_4d\zeta_4, \tag{4}$$

where $\psi(\boldsymbol{r}\zeta)$ and $\psi^\dagger(\boldsymbol{r}\zeta)$ are field operators of electrons, and $\boldsymbol{r}$ and ζ are spatial and spin coordinates, respectively. In Eqs. (1) and (4), $\hat{\Delta}(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$, $\hat{n}(\boldsymbol{r})$, $\hat{\boldsymbol{j}}_p^{(T)}(\boldsymbol{r})$, and $\hat{\boldsymbol{j}}_{M_s}(\boldsymbol{r})$ denote operators of the OPSS [27,43], electron density, transverse component of the paramagnetic-current density [27,44], and spin current density [44], respectively. They are defined by

$$\hat{\Delta}(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2) = \psi(\boldsymbol{r}_2\zeta_2)\psi(\boldsymbol{r}_1\zeta_1), \tag{5}$$

$$\hat{n}(\boldsymbol{r}) = \int \psi^\dagger(\boldsymbol{r}\zeta)\psi(\boldsymbol{r}\zeta)d\zeta, \tag{6}$$

$$\hat{\boldsymbol{j}}_p^{(T)}(\boldsymbol{r}) = \frac{\hbar}{4\pi i m}\int\{\nabla_{\boldsymbol{r}'}\psi^\dagger(\boldsymbol{r}'\zeta')\times\nabla_{\boldsymbol{r}'}\psi(\boldsymbol{r}'\zeta')\} \times\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}d^3r'd\zeta', \tag{7}$$

$$\hat{\boldsymbol{j}}_{M_s}(\boldsymbol{r}) = g\frac{\mu_B}{e\hbar}\nabla\times\int\psi^\dagger(\boldsymbol{r}\zeta)\hat{\boldsymbol{s}}_{op}^{\zeta}\psi(\boldsymbol{r}\zeta)d\zeta, \tag{8}$$

where g and μ_B are the g factor ($g = 2.0023$) and Bohr magneton ($\mu_B = e\hbar/2m$), respectively, and $\hat{\boldsymbol{s}}_{op}^{\zeta}$ is the usual operator of spin. The first, second, and third terms of Eq. (1) are operators of the kinetic energy, electron-electron interaction energy, and attractive interaction energy via $w(\boldsymbol{r}_1\zeta_1\boldsymbol{r}_2\zeta_2;\boldsymbol{r}_3\zeta_3\boldsymbol{r}_4\zeta_4)$, respectively [27]. The vector potential $\boldsymbol{A}_{\rm given}(\boldsymbol{r})$ denotes a before-given electromagnetic field that is determined by the microscopic Maxwell equation [27], and the Coulomb gauge is adopted to $\boldsymbol{A}_{\rm given}(\boldsymbol{r})$. The fourth term of Eq. (1) is the interaction between the vector potential and paramagnetic-current density [27]. The fifth term of Eq. (1) denotes the spin-Zeeman effect. Note that the fourth and sixth terms denote the effects of currents that are not considered in Spin-SCDFT [21,22]. Hereafter, we denote the statistical averages of $\hat{\Delta}(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$, $\hat{n}(\boldsymbol{r})$, $\hat{\boldsymbol{j}}_p^{(T)}(\boldsymbol{r})$, and $\hat{\boldsymbol{j}}_{M_s}(\boldsymbol{r})$ by $\Delta(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$, $n(\boldsymbol{r})$, $\boldsymbol{j}_p^{(T)}(\boldsymbol{r})$, and $\boldsymbol{j}_{M_s}(\boldsymbol{r})$, respectively.

In the present theory, $n(\boldsymbol{r})$, $\boldsymbol{j}_p^{(T)}(\boldsymbol{r})$, $\boldsymbol{j}_{M_s}(\boldsymbol{r})$, $\Delta(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$, and $\Delta^*(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$ are chosen as basic variables. In comparison with the previous theory [27], $\boldsymbol{j}_{M_s}(\boldsymbol{r})$ is added into the member of basic variables due to the incorporation of the spin-Zeeman effect into the Hamiltonian. In a way similar to the previous theory [27], we define the universal energy functional as

$$F\left[n,\boldsymbol{j}_p^{(T)},\boldsymbol{j}_{M_s},\Delta,\Delta^*\right] = \mathop{\rm Min}_{\hat{\rho}\to(n,\boldsymbol{j}_p^{(T)},\boldsymbol{j}_{M_s},\Delta,\Delta^*)}{\rm Tr}\left\{\hat{\rho}(\hat{T}+\hat{W}_1+\hat{W}_2)+\frac{1}{\beta}\hat{\rho}\ln\hat{\rho}\right\}, \tag{9}$$

where $\hat{\rho}$ denotes the statistical operator. The right-hand side of Eq. (9) means that the minimum value of the statistical average of $\hat{T}+\hat{W}_1+\hat{W}_2$ plus entropy-related term is searched within the set of statistical density operators that yield prescribed (n, $\boldsymbol{j}_p^{(T)}$, $\boldsymbol{j}_{M_s}$, Δ, Δ^*). The extended Hohenberg-Kohn (HK) theorem can be proved by means of this universal energy functional. The extended HK theorem consists of the following two theorems. (I) One is the variational principle with respect to basic variables. This variational principle can be derived by rewriting Gibbs's variational principle. (II) The other is a one-to-one correspondence between the correct density operator and basic variables for the equilibrium state. The details of the proof of the extended HK theorem are given in the previous paper [27] for the case where $n(\boldsymbol{r})$, $\boldsymbol{j}_p^{(T)}(\boldsymbol{r})$, $\Delta(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$, and $\Delta^*(\boldsymbol{r}_1\zeta_1,\boldsymbol{r}_2\zeta_2)$ are chosen as basic variables. Also for the present case, the extended HK theorem can be proved in a similar way as the previous case [27].

We introduce the noninteracting system as the reference system, in which basic variables for the equilibrium state of the real system are reproduced. The Hamiltonian of the reference system is supposed to be given by

$$\hat{H}_s = \int\psi^\dagger(\boldsymbol{r}\zeta)\left[\frac{1}{2m}\{\boldsymbol{p}+e\boldsymbol{A}_s(\boldsymbol{r})\}^2\right]\psi(\boldsymbol{r}\zeta)d^3rd\zeta + \int v_s(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}\zeta)\psi(\boldsymbol{r}\zeta)d^3rd\zeta + e\int\hat{\boldsymbol{j}}_{M_s}(\boldsymbol{r})\cdot\boldsymbol{A}_s(\boldsymbol{r}t)d^3r + \iint D_s^*(\boldsymbol{r}\zeta\boldsymbol{r}'\zeta')\hat{\Delta}(\boldsymbol{r}\zeta\boldsymbol{r}'\zeta')d^3rd\zeta d^3r'd\zeta' + \iint D_s(\boldsymbol{r}\zeta\boldsymbol{r}'\zeta')\hat{\Delta}^\dagger(\boldsymbol{r}\zeta\boldsymbol{r}'\zeta')d^3rd\zeta d^3r'd\zeta', \tag{10}$$

where $v_s(\boldsymbol{r})$, $\boldsymbol{A}_s(\boldsymbol{r})$, $D_s(\boldsymbol{r}\zeta\boldsymbol{r}'\zeta')$, and $D_s^*(\boldsymbol{r}\zeta\boldsymbol{r}'\zeta')$ are effective mean-field potentials. If the universal energy functional of the reference system is defined by

$$F_s\left[n,\boldsymbol{j}_p^{(T)},\boldsymbol{j}_{M_s},\Delta,\Delta^*\right] = \mathop{\rm Min}_{\hat{\rho}\to(n,\boldsymbol{j}_p^{(T)},\boldsymbol{j}_{M_s},\Delta,\Delta^*)}{\rm Tr}\left\{\hat{\rho}\hat{T}+\frac{1}{\beta}\hat{\rho}\ln\hat{\rho}\right\}, \tag{11}$$

then we can prove the extended HK theorem for the reference system in a similar way to the case of the real system.

The effective potentials are determined by using the extended HK theorems for the real and reference systems so that the basic variables for the equilibrium state of the real system

are reproduced in the reference system [27]. The concrete expressions of effective potentials are given by

$$v_s(\boldsymbol{r}) = v_{\rm ext}(\boldsymbol{r}) + e^2 \int \frac{n_0(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} d^3r' + \left.\frac{\delta F_{xc}\left[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\right]}{\delta n(\boldsymbol{r})}\right|_{\substack{n=n_0 \\ \boldsymbol{j}_p^{(T)}=\boldsymbol{j}_{p0}^{(T)} \\ \boldsymbol{j}_{Ms}=\boldsymbol{j}_{Ms0} \\ \Delta=\Delta_0 \\ \Delta^*=\Delta_0^*}} + \frac{e^2}{2m}\left\{\boldsymbol{A}_{\rm given}^2(\boldsymbol{r}) - \boldsymbol{A}_s^2(\boldsymbol{r})\right\}, \tag{12}$$

$$\boldsymbol{A}_s(\boldsymbol{r}) = \boldsymbol{A}_{\rm given}(\boldsymbol{r}) + \frac{1}{e}\left.\frac{\delta F_{xc}[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*]}{\delta \boldsymbol{j}_p^{(T)}(\boldsymbol{r})}\right|_{\substack{n=n_0 \\ \boldsymbol{j}_p^{(T)}=\boldsymbol{j}_{p0}^{(T)} \\ \boldsymbol{j}_{Ms}=\boldsymbol{j}_{Ms0} \\ \Delta=\Delta_0 \\ \Delta^*=\Delta_0^*}}, \tag{13}$$

$$D_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = \left.\frac{\delta F_{xc}\left[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\right]}{\delta \Delta^*(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')}\right|_{\substack{n=n_0 \\ \boldsymbol{j}_p^{(T)}=\boldsymbol{j}_{p0}^{(T)} \\ \boldsymbol{j}_{Ms}=\boldsymbol{j}_{Ms0} \\ \Delta=\Delta_0 \\ \Delta^*=\Delta_0^*}}, \tag{14}$$

$$D_s^*(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = \left.\frac{\delta F_{xc}\left[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\right]}{\delta \Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')}\right|_{\substack{n=n_0 \\ \boldsymbol{j}_p^{(T)}=\boldsymbol{j}_{p0}^{(T)} \\ \boldsymbol{j}_{Ms}=\boldsymbol{j}_{Ms0} \\ \Delta=\Delta_0 \\ \Delta^*=\Delta_0^*}}, \tag{15}$$

where n_0, $\boldsymbol{j}_{p0}^{(T)}$, $\boldsymbol{j}_{Ms0}$, Δ_0, and Δ_0^* are the basic variables for the equilibrium state of the system. The energy functional $F_{xc}[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*]$ that appears in Eqs. (12)–(15) denotes the exchange-correlation energy functional of the present theory. This functional is defined by

$$F_{xc}\left[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\right] = F\left[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\right] - F_s\left[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\right] - \frac{e^2}{2}\iint \frac{n(\boldsymbol{r})n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} d^3r d^3r'. \tag{16}$$

To perform actual calculations, the approximate form of $F_{xc}[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*]$ is indispensable. The approximate form will be proposed in the next subsection.

The Hamiltonian of the reference system $\hat{H}_s$ can be diagonalized in terms of the fermion quasiparticle via the Bogoliubov-Valatin (BV) transformation [45,46]. The transformation is supposed to be given by

$$\psi(\boldsymbol{r}\zeta) = \sum_{\boldsymbol{k}} u_{\boldsymbol{k}}(\boldsymbol{r}\zeta)\gamma_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} v_{\boldsymbol{k}}(\boldsymbol{r}\zeta)\gamma_{\boldsymbol{k}}^\dagger,$$
$$\psi^\dagger(\boldsymbol{r}\zeta) = \sum_{\boldsymbol{k}} u_{\boldsymbol{k}}^*(\boldsymbol{r}\zeta)\gamma_{\boldsymbol{k}}^\dagger + \sum_{\boldsymbol{k}} v_{\boldsymbol{k}}^*(\boldsymbol{r}\zeta)\gamma_{\boldsymbol{k}}, \tag{17}$$

where $\gamma_{\boldsymbol{k}}$ and $\gamma_{\boldsymbol{k}}^\dagger$ denote annihilation and creation operators of the fermion quasiparticles, and $u_{\boldsymbol{k}}(\boldsymbol{r}\zeta)$ and $v_{\boldsymbol{k}}(\boldsymbol{r}\zeta)$ correspond to the matrix elements of the BV transformation. They are determined by requiring $\hat{H}_s$ to be diagonalized in terms of $\gamma_{\boldsymbol{k}}$ and $\gamma_{\boldsymbol{k}}^\dagger$ [27]. As a result, we obtain the Bogoliubov–de Gennes (BdG)–Kohn-Sham (KS) equation for $u_{\boldsymbol{k}}(\boldsymbol{r}\zeta)$ and $v_{\boldsymbol{k}}(\boldsymbol{r}\zeta)$ in a way similar to the case of the previous paper [27]:

$$\begin{aligned}
&\left(h_s^r - \mu\right)u_{\boldsymbol{k}}(\boldsymbol{r}\zeta) + \int \tilde{D}_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')v_{\boldsymbol{k}}^*(\boldsymbol{r}'\zeta')d\boldsymbol{r}'d\zeta' \\
&\quad = E_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r}\zeta) \\
&-\left(h_s^r - \mu\right)v_{\boldsymbol{k}}(\boldsymbol{r}\zeta) + \int \tilde{D}_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')u_{\boldsymbol{k}}^*(\boldsymbol{r}'\zeta')d\boldsymbol{r}'d\zeta' \\
&\quad = E_{\boldsymbol{k}}v_{\boldsymbol{k}}(\boldsymbol{r}\zeta),
\end{aligned} \tag{18}$$

with

$$h_s^r = \frac{\{\boldsymbol{p} + e\boldsymbol{A}_s(\boldsymbol{r})\}^2}{2m} + v_s(\boldsymbol{r}) + g\frac{\mu_B}{\hbar}\hat{\boldsymbol{s}}_{op}^\zeta \cdot \boldsymbol{B}_s(\boldsymbol{r}), \tag{19}$$

$$\tilde{D}_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = D_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') - D_s(\boldsymbol{r}'\zeta', \boldsymbol{r}\zeta), \tag{20}$$

where $\boldsymbol{B}_s(\boldsymbol{r}) = \nabla \times \boldsymbol{A}_s(\boldsymbol{r})$. The basic variables are reproduced by means of the solution of the BdG–KS equation as follows:

$$n_0(\boldsymbol{r}) = \sum_{\boldsymbol{k}} f(E_{\boldsymbol{k}}) \int |u_{\boldsymbol{k}}(\boldsymbol{r}\zeta)|^2 d\zeta + \sum_{\boldsymbol{k}} \{1 - f(E_{\boldsymbol{k}})\} \int |v_{\boldsymbol{k}}(\boldsymbol{r}\zeta)|^2 d\zeta, \tag{21}$$

$$\boldsymbol{j}_{p0}^{(T)}(\boldsymbol{r}) = \frac{\hbar}{i4\pi m}\sum_{\boldsymbol{k}}\left[f(E_{\boldsymbol{k}})\int \{\nabla_{\boldsymbol{r}'}u_{\boldsymbol{k}}^*(\boldsymbol{r}'\zeta') \times \nabla_{\boldsymbol{r}'}u_{\boldsymbol{k}}(\boldsymbol{r}'\zeta')\} \times \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}d^3r'd\zeta + \{1 - f(E_{\boldsymbol{k}})\}\int \left\{\nabla_{\boldsymbol{r}'}v_{\boldsymbol{k}}^*(\boldsymbol{r}'\zeta') \times \nabla_{\boldsymbol{r}'}v_{\boldsymbol{k}}(\boldsymbol{r}'\zeta')\right\} \times \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|^3}d^3r'd\zeta\right], \tag{22}$$

$$\boldsymbol{j}_{Ms0}(\boldsymbol{r}) = g\frac{\mu_B}{e\hbar}\nabla \times \int \sum_{\boldsymbol{k}}\left[f(E_{\boldsymbol{k}})u_{\boldsymbol{k}}^*(\boldsymbol{r}\zeta)\hat{\boldsymbol{s}}_{op}^\zeta u_{\boldsymbol{k}}(\boldsymbol{r}\zeta) + \{1 - f(E_{\boldsymbol{k}})\}v_{\boldsymbol{k}}^*(\boldsymbol{r}\zeta)\hat{\boldsymbol{s}}_{op}^\zeta v_{\boldsymbol{k}}(\boldsymbol{r}\zeta)\right]d\zeta, \tag{23}$$

$$\Delta_0(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = \frac{1}{2}\sum_{\boldsymbol{k}}\{u_{\boldsymbol{k}}(\boldsymbol{r}'\zeta')v_{\boldsymbol{k}}(\boldsymbol{r}\zeta) - v_{\boldsymbol{k}}(\boldsymbol{r}'\zeta')u_{\boldsymbol{k}}(\boldsymbol{r}\zeta)\}\{1 - 2f(E_{\boldsymbol{k}})\}, \tag{24}$$

$$\Delta_0^*(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = \frac{1}{2}\sum_{\boldsymbol{k}}\{u_{\boldsymbol{k}}^*(\boldsymbol{r}'\zeta')v_{\boldsymbol{k}}^*(\boldsymbol{r}\zeta) - v_{\boldsymbol{k}}^*(\boldsymbol{r}'\zeta')u_{\boldsymbol{k}}^*(\boldsymbol{r}\zeta)\}\{1 - 2f(E_{\boldsymbol{k}})\}, \tag{25}$$

where $f(E_k)$ denotes the Fermi-Dirac distribution function and is given by $1/(e^{\beta E_k}+1)$.

The calculation procedure is similar to the previous theory [27]. For a before-given electromagnetic field $\boldsymbol{A}_{\rm given}(\boldsymbol{r})$ (input electromagnetic field), Eqs. (12)–(15) and (18)–(25) are solved in a self-consistent way. Then we obtain the electron density and current density by using thus obtained basic variables [27]. By using the electron density and current density, the electromagnetic field is calculated by solving the microscopic Maxwell equation. Comparing the thus obtained electromagnetic field with the input one, if they are not consistent with each other, then the input electromagnetic field is changed until the self-consistency is attained within some accuracy [27].

B. Gap equation for superconductors immersed in a magnetic field

To implement numerical calculations based on the CDFT for superconductors, we need the approximate form of the exchange-correlation energy functional, the definition of which is given by Eq. (16). In this study, we assume the following approximate form that induces the OPSS with spin-singlet symmetry:

$$\begin{aligned} &F_{xc}\big[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms},\, \Delta,\, \Delta^*\big] \\ &\quad = E_{xc}\big[n,\, \boldsymbol{j}_p^T,\, \boldsymbol{j}_{Ms}\big] + \frac{1}{2}\iint \Delta^*(\boldsymbol{r}_1\zeta_1, \boldsymbol{r}_2\zeta_2) \\ &\qquad \times w(\boldsymbol{r}_1\zeta_1, \boldsymbol{r}_2\zeta_2; \boldsymbol{r}_3\zeta_3, \boldsymbol{r}_4\zeta_4) \\ &\qquad \times \Delta(\boldsymbol{r}_4\zeta_4, \boldsymbol{r}_3\zeta_3) d\boldsymbol{r}_1 d\zeta_1 d\boldsymbol{r}_2 d\zeta_2 d\boldsymbol{r}_3 d\zeta_3 d\boldsymbol{r}_4 d\zeta_4, \end{aligned} \tag{26}$$

with

$$\begin{aligned} &w(\boldsymbol{r}_1\zeta_1, \boldsymbol{r}_2\zeta_2; \boldsymbol{r}_3\zeta_3, \boldsymbol{r}_4\zeta_4) \\ &\quad = -V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_4)\delta(\boldsymbol{r}_2 - \boldsymbol{r}_3)\langle\zeta_1|\sigma_y|\zeta_2\rangle\langle\zeta_4|\sigma_y|\zeta_3\rangle. \end{aligned} \tag{27}$$

The first term on the right-hand side of Eq. (26) denotes a part of the exchange-correlation energy functional that is independent of the OPSS. The second term has a form that is obtained from the expectation value of the attractive interaction energy ($\hat{W}_2$) under the mean-field approximation. In this approximation, the effective pair potential $\tilde{D}_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')$ can be obtained by using Eqs. (14), (15), and (20). We have

$$\tilde{D}_s(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = iV(|\boldsymbol{r} - \boldsymbol{r}'|)\bar{\Delta}(\boldsymbol{r}, \boldsymbol{r}')\langle\zeta|\sigma_y|\zeta'\rangle, \tag{28}$$

with

$$\bar{\Delta}(\boldsymbol{r}, \boldsymbol{r}') = \frac{1}{i}\iint \Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')\langle\zeta|\sigma_y|\zeta'\rangle d\zeta d\zeta'. \tag{29}$$

Here, $\langle\zeta|\sigma_y|\zeta'\rangle$ is given by $i\{\chi_\downarrow(\zeta)\chi_\uparrow(\zeta') - \chi_\uparrow(\zeta)\chi_\downarrow(\zeta')\}$, where $\chi_\sigma(\zeta)$ denotes the spin function, and $\bar{\Delta}(\boldsymbol{r}, \boldsymbol{r}')$ denote a the singlet part of $\Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')$.

To solve the BdG–KS equation, we adopt the approximation method presented by de Gennes [47]. He introduced one-electron wave functions in the normal state when solving the BdG equation [47], and assumed that the solutions of the BdG equation have the same spatial dependence as the one-electron wave functions [47]. Similar to this approximation method, the solution of the BdG–KS equation is determined in the following form:

$$\begin{aligned} u_k(\boldsymbol{r}\zeta) &= \bar{u}_k w_{k\downarrow}(\boldsymbol{r})\chi_\downarrow(\zeta), \\ v_k(\boldsymbol{r}\zeta) &= \bar{v}_k w_{k\uparrow}(\boldsymbol{r})\chi_\uparrow(\zeta), \end{aligned} \tag{30}$$

where $w_{k\sigma}(\boldsymbol{r})\chi_\sigma(\zeta)$ denotes the KS orbital of the normal state that is defined as the eigenfunction of $h_s^r - \mu$:

$$\big(h_s^r - \mu\big)w_{k\sigma}(\boldsymbol{r})\chi_\sigma(\zeta) = \xi_{k\sigma} w_{k\sigma}(\boldsymbol{r})\chi_\sigma(\zeta). \tag{31}$$

Substituting Eqs. (28) and (30) into Eq. (18), and using Eq. (31), the BdG–KS equation can be rewritten as

$$\begin{bmatrix} \xi_{k\downarrow} & i\Gamma_k(B_s, T) \\ -i\Gamma_k(B_s, T) & -\xi_{k\uparrow} \end{bmatrix}\begin{bmatrix} \bar{u}_k \\ \bar{v}_k^* \end{bmatrix} = E_k \begin{bmatrix} \bar{u}_k \\ \bar{v}_k^* \end{bmatrix}, \tag{32}$$

with

$$\Gamma_k(B_s, T) = i\iint w_{k\downarrow}^*(\boldsymbol{r})V(|\boldsymbol{r} - \boldsymbol{r}'|)\bar{\Delta}(\boldsymbol{r}, \boldsymbol{r}')w_{k\uparrow}^*(\boldsymbol{r}')d\boldsymbol{r}d\boldsymbol{r}'. \tag{33}$$

By solving Eq. (32), we have

$$E_k = \sqrt{\bar{\xi}_k^2 + |\Gamma_k(B_s, T)|^2} - \frac{\Delta\xi_k}{2}, \tag{34}$$

$$|\bar{u}_k|^2 = \frac{1}{2}\left\{1 + \frac{\bar{\xi}_k}{\sqrt{\bar{\xi}_k^2 + |\Gamma_k(B_s, T)|^2}}\right\}, \tag{35}$$

$$|\bar{v}_k|^2 = \frac{1}{2}\left\{1 - \frac{\bar{\xi}_k}{\sqrt{\bar{\xi}_k^2 + |\Gamma_k(B_s, T)|^2}}\right\}, \tag{36}$$

where $\Delta\xi_k = \xi_{k\uparrow} - \xi_{k\downarrow}$ and $\bar{\xi}_k = (\xi_{k\uparrow} + \xi_{k\downarrow})/2$. Equation (34) implies that the energy gap $\Gamma_k(B_s, T)$ appears in the energy spectrum of the superconducting state. It should be noted that E_k, $|\bar{u}_k|^2$, and $|\bar{v}_k|^2$ are reduced to $\sqrt{\xi_k^2 + |\Gamma_k(0, T)|^2}$, $\{1 + \xi_k/E_k\}/2$, and $\{1 - \xi_k/E_k\}/2$ in the limit of $\boldsymbol{B}_s(\boldsymbol{r}) \to 0$ and $v_{\rm ext}(\boldsymbol{r}) \to$ const. (homogeneous limit), where ξ_k denotes the eigenvalue of the normal state in the zero-magnetic-field case. These expressions in the limit are identical to those of the Bardeen-Cooper-Schrieffer (BCS) theory [48], which implies that the present scheme is reasonable because it covers the BCS theory as the limiting case.

Substituting Eq. (30) into Eq. (24), and using Eq. (29), we have

$$\bar{\Delta}(\boldsymbol{r}, \boldsymbol{r}') = \sum_k \bar{u}_k\bar{v}_k w_k(\boldsymbol{r})w_k(\boldsymbol{r}')\tanh\left\{\frac{\beta}{2}E_k\right\}. \tag{37}$$

Substituting Eq. (37) into Eq. (33), and using Eqs. (35) and (36), we have

$$\begin{aligned} \Gamma_k(B_s, T) = \frac{1}{2}\sum_{k'} &\frac{V_{kk'}\Gamma_{k'}(B_s, T)}{\sqrt{\bar{\xi}_{k'}^2 + |\Gamma_{k'}(B_s, T)|^2}} \\ &\times \tanh\left\{\frac{\beta}{2}\left[\sqrt{\bar{\xi}_{k'}^2 + |\Gamma_{k'}(B_s, T)|^2} - \frac{\Delta\xi_{k'}}{2}\right]\right\}, \end{aligned} \tag{38}$$

with

$$V_{kk'} = \frac{1}{2}\iint w^*_{k\downarrow}(\boldsymbol{r})w^*_{k\uparrow}(\boldsymbol{r}')V(|\boldsymbol{r}-\boldsymbol{r}'|)w_{k'\uparrow}(\boldsymbol{r})w_{k'\downarrow}(\boldsymbol{r}') \times d^3\boldsymbol{r}d^3\boldsymbol{r}' + \frac{1}{2}\iint w^*_{k\downarrow}(\boldsymbol{r})w^*_{k\uparrow}(\boldsymbol{r}') \times V(|\boldsymbol{r}-\boldsymbol{r}'|)w_{k'\downarrow}(\boldsymbol{r})w_{k'\uparrow}(\boldsymbol{r}')d^3\boldsymbol{r}d^3\boldsymbol{r}'. \quad (39)$$

Equation (38) is regarded as the gap equation for superconductors immersed in a magnetic field. If $\Gamma_{\boldsymbol{k}}(B_s, T)$ is obtained by solving Eq. (38), then $u_{\boldsymbol{k}}(\boldsymbol{r}\zeta)$ and $v_{\boldsymbol{k}}(\boldsymbol{r}\zeta)$ are calculated by using Eqs. (30) and (34)–(36). Therefore, the basic variables are calculated by using Eqs. (21)–(25). Thus, by employing approximation Eqs. (26) and (30), the problem of solving the BdG–KS equation [Eq. (18)] is reduced to that of solving the gap equation [Eq. (38)].

Similarly to the BCS theory, the matrix elements of the attractive interaction $V_{kk'}$ are assumed to be nonzero and constant (V_0) for the electrons inside the energy region ($\bar{\xi}_{\boldsymbol{k}} < \hbar\omega_D$) near the Fermi energy, where ω_D denotes the Debye frequency. In this case, it is reasonable to assume that $\Gamma_{\boldsymbol{k}}(B_s, T)$ is independent of $\boldsymbol{k}$ in a similar way to the BCS theory [48]. Furthermore, $\Delta\xi_{\boldsymbol{k}}$ is supposed to be independent of $\boldsymbol{k}$ because the splitting $\Delta\xi_{\boldsymbol{k}}$ is mainly caused by the spin-Zeeman effect. The summation with respect to $\boldsymbol{k}'$ in Eq. (38) can be rewritten as an integral with respect to the energy by using the density of state (DOS). In this case, the gap equation is reduced to

$$1 = V_0 D(0)\int_0^{\hbar\omega_D} \frac{\tanh\left\{\frac{\beta}{2}\left[\sqrt{\xi^2+|\Gamma_0(B_s,T)|^2}-\frac{\Delta\xi}{2}\right]\right\}}{\sqrt{\xi^2+|\Gamma_0(B_s,T)|^2}}d\xi, \quad (40)$$

where $D(0)$ denotes the DOS for $\bar{\xi}_{\boldsymbol{k}}$ at the Fermi energy. Here, $\Gamma_{\boldsymbol{k}}(B_s, T)$ and $\Delta\xi_{\boldsymbol{k}}$ are denoted as $\Gamma_0(B_s, T)$ and $\Delta\xi$, respectively. It is confirmed that Eq. (40) is reduced to the gap equation of the BCS theory [48] in the limit of $\boldsymbol{B}_s(\boldsymbol{r}) \to 0$ and $v_{\rm ext}(\boldsymbol{r}) \to$ const. (homogeneous limit), which implies the validity of the approximation.

III. PRACTICAL SCHEME FOR SOLVING THE GAP EQUATION

To validate the proposed gap equation, we apply it to aluminum immersed in a magnetic field. For this purpose, we consider homogeneous electron gas immersed in a magnetic field. The value of r_s, which stands for the average distance between electrons, of the homogeneous electron gas is 2.07 for aluminum [49]. The external magnetic field is supposed to be parallel to the z axis. In the present calculations, we neglect $E_{xc}[n, \boldsymbol{j}_p^T, \boldsymbol{j}_{M_S}]$ [50], which is independent of the OPSS [Eq. (26)] and denotes the exchange-correlation effects of the electron-electron interaction. Because the potential energy caused by the positive background charge is canceled out by the Hartree potential, we have $v_s(\boldsymbol{r}) \approx 0$ and $\boldsymbol{A}_s(\boldsymbol{r}) \approx \boldsymbol{A}_{\rm given}(\boldsymbol{r})$ under these approximations. Although the profile of $\boldsymbol{A}_{\rm given}(\boldsymbol{r})$ is determined by solving the gap equation and microscopic Maxwell equation simultaneously as mentioned in the previous section, we suppose that the thus obtained $\boldsymbol{A}_{\rm given}(\boldsymbol{r})$ is given by

$$\boldsymbol{A}_{\rm given}(\boldsymbol{r}) = \left[0,\ \lambda\bar{B}\sinh\left(\frac{x}{2\lambda}\right), 0\right], \quad (41)$$

with $\bar{B} = B_{\rm ext}/\cosh(L_x/2\lambda)$, where λ and $B_{\rm ext}$ denote the magnetic penetration depth and the magnitude of the external magnetic field, respectively. Hereafter, we denote the magnetic-field dependence of the superconducting gap as $\Gamma_0(B_{\rm ext}, T)$ instead of $\Gamma_0(B_s, T)$, because of Eq. (41). By using $v_s(\boldsymbol{r}) \approx 0$ as previously discussed, and Eq. (41), we calculate the KS orbital of the normal state and eigenvalue of Eq. (31).

Although the magnetic-field-containing relativistic tight-binding approximation (MFRTB) method [51–56] is useful for calculating the electronic structure of materials immersed in a uniform magnetic field, the magnetic field is nonuniform in this case [Eq. (41)]. Therefore, we employ the perturbation theory in the present calculations. Specifically, the magnetic-field-dependent terms in h_s^r, which are given by $\frac{e}{2m}\{\boldsymbol{p}\cdot\boldsymbol{A}_s(\boldsymbol{r}) + \boldsymbol{A}_s(\boldsymbol{r})\cdot\boldsymbol{p}\}$, $\frac{e^2\boldsymbol{A}_s(\boldsymbol{r})^2}{2m}$, and $g\frac{\mu_B}{\hbar}\hat{\boldsymbol{s}}^\zeta_{op}\cdot\boldsymbol{B}_s(\boldsymbol{r})$, are treated as the perturbation. We calculate the eigenvalue $\xi_{\boldsymbol{k}\sigma}$ and the DOS by considering the first and second order of $B_{\rm ext}$.

To perform the above-mentioned calculations, the value of λ should be determined appropriately. For this, we use the following relation:

$$2n^{(2)}_{\rm max}(B_{\rm ext}, T)\Gamma_0(B_{\rm ext}, T) = 2n^{(2)}_{\rm max}(0, T)\Gamma_0(0, T) - \frac{B^2_{\rm ext}}{2\mu_0}\Omega, \quad (42)$$

where $2n^{(2)}_{\rm max}(B_{\rm ext}, T)$ is the number of superconducting electrons [43]. The left-hand side of this equation denotes the energy gain obtained in the superconducting state (the superconducting energy gain in the presence of the magnetic field), and the right-hand side suggests that the superconducting energy gain in the absence of the magnetic field is reduced because of the diamagnetic potential energy caused by the Meissner effect. This equation corresponds to Ittner's relation [57], if λ is considerably smaller than the thickness of the superconductor and if the magnitude of the magnetic field approaches the critical magnetic field. Therefore, the calculation properties that will be presented in Sec. IV correspond to those of the bulk system. The value of $2n^{(2)}_{\rm max}(B_{\rm ext}, T)$ can be calculated from $\Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')$ in the present scheme. Since the occupation number of a two-particle state becomes an order N in the superconducting state, $\Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')$ can be described by [43]

$$\Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta') = \sqrt{2n^{(2)}_{\rm max}(B_{\rm ext}, T)}\nu_{\rm max}(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta'), \quad (43)$$

where $\nu_{\rm max}(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')$ denotes the two-particle state. This equation leads to $2n^{(2)}_{\rm max}(B_{\rm ext}, T) = \iint|\Delta(\boldsymbol{r}\zeta, \boldsymbol{r}'\zeta')|^2 d^3\boldsymbol{r}d^3\boldsymbol{r}'d\zeta d\zeta'$. By using Eqs. (24), (30), (35), and (36), we have

$$\begin{aligned} 2n^{(2)}_{\rm max}(B_{\rm ext}, T) &= \frac{1}{8}\sum_{k'}\frac{|\Gamma_{k'}(B_{\rm ext}, T)|^2}{\bar{\xi}^2_{k'} + |\Gamma_{k'}(B_{\rm ext}, T)|^2} \times \tanh^2\left\{\frac{\beta}{2}\left[\sqrt{\bar{\xi}^2_{k'} + |\Gamma_{k'}(B_{\rm ext}, T)|^2} - \frac{\Delta\xi_{k'}}{2}\right]\right\} \\ &\approx \frac{D(0)}{4}\int_0^{\hbar\omega_D}\frac{|\Gamma_0(B_{\rm ext}, T)|^2}{\xi^2 + |\Gamma_0(B_{\rm ext}, T)|^2} \times \tanh^2\left\{\frac{\beta}{2}\left[\sqrt{\xi^2 + |\Gamma_0(B_{\rm ext}, T)|^2} - \frac{\Delta\xi}{2}\right]\right\}d\xi. \end{aligned} \quad (44)$$

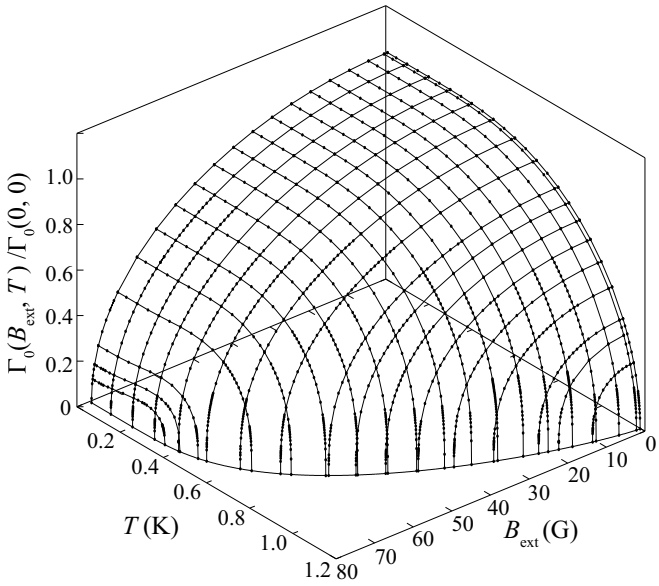

FIG. 1. Dependence of the superconducting gap on the temperature and magnetic field.

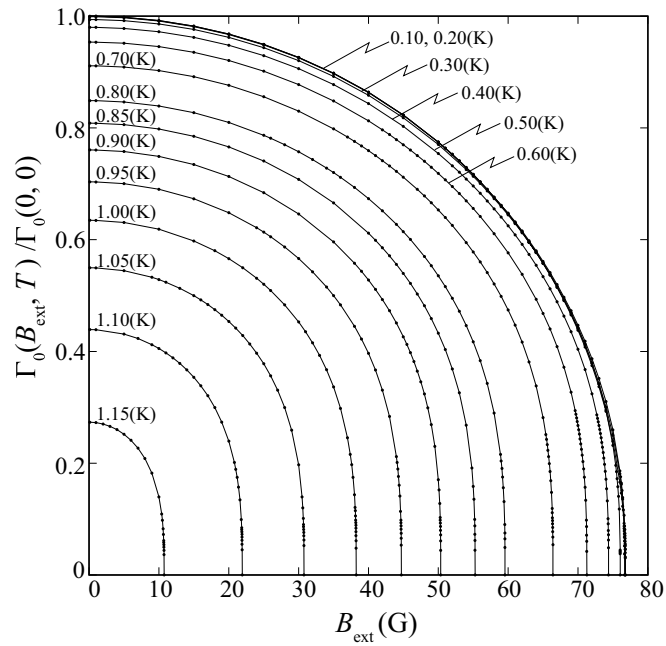

FIG. 2. Magnetic-field dependence of the superconducting gap for fixed temperature.

By solving the gap equation [Eq. (40)] simultaneously with Eq. (44), we can obtain $\Gamma_0(B_{\rm ext}, T)$ and λ. This practical scheme enables us to solve the gap equation without solving the microscopic Maxwell equation simultaneously.

The procedure of numerical calculations is as follows. First, we calculate $D(0)$ for a trial value of λ by means of the perturbation theory. Then, we solve the gap equation [(Eq. (40)] by using the obtained $D(0)$, and get $\Gamma_0(B_{\rm ext}, T)$. By means of Eq. (44), $2n^{(2)}_{\rm max}(B_{\rm ext}, T)$ can be calculated by using $D(0)$ and $\Gamma_0(B_{\rm ext}, T)$. By substituting the values of $2n^{(2)}_{\rm max}(B_{\rm ext}, T)$ and $\Gamma_0(B_{\rm ext}, T)$ into Eq. (42), we can check whether Eq. (42) is satisfied or not. If not, the value of λ is changed appropriately. This procedure is performed until Eq. (42) holds.

In actual calculations, the value of V_0 is assumed to be the same as that for the zero-magnetic-field case. We employ the unperturbed KS orbital to calculate the matrix elements of the attractive interaction. Specifically, the value of V_0 is determined by using the formula for the critical temperature [48], $k_B T_c \approx 1.134\hbar\omega_D \exp[-1/V_0\bar{N}(0)]$, where $\bar{N}(0)$ denotes the DOS at the Fermi energy for the zero magnetic field. This formula is obtained by the BCS theory. We use $V_0\bar{N}(0) = 0.1661$. The value is obtained by using $T_c = 1.18$ K for aluminum and $\omega_D = k_B\theta_D/\hbar$ with the Debye temperature $\theta_D = 428$ K for aluminum [58]. For the value of $\bar{N}(0)$, we use the DOS of the homogeneous electron with $r_s = 2.07$ [49]. We consider a rectangular system with the dimensions $L_x = 1$ cm, $L_y = 10$ cm, and $L_z = 10$ cm.

IV. CALCULATION RESULTS AND DISCUSSION

Figure 1 shows the dependence of the superconducting gap on the temperature and magnetic field. The z axis denotes the ratio $\Gamma_0(B_{\rm ext}, T)/\Gamma_0(0, 0)$, where $\Gamma_0(0, 0)$ is calculated as 0.1793 eV by Eq. (40). This value of $\Gamma_0(0, 0)$ is consistent with the literature data [58]. Thus, the present scheme enables us to predict the temperature and magnetic-field dependences of the superconducting gap. This is a prediction of the magnetic-field and temperature dependence of the superconducting gap on the basis of the first-principles calculation method, i.e., the CDFT for superconductors. In the following, we discuss this dependence in detail.

The projection of this three-dimensional plot (Fig. 1) onto the $T = 0$ plane is shown in Fig. 2. The gap $\Gamma_0(B_{\rm ext}, T)$ monotonically decreases with the magnetic field and is convex upward. The critical magnetic field is defined as the magnetic field at which the superconducting gap disappears. The obtained value of B_c is approximately 76.79 G at $T = 0.01$ K. This value is in reasonably good agreement with the experimental result ($B_c = 99$ G) [59].

The projection of Fig. 1 onto the $B_{\rm ext} = 0$ plane is shown in Fig. 3. The critical temperature is also defined as the temperature at which the superconducting gap disappears. The critical temperature decreases with an increase in the magnetic field. The critical temperature at $B_{\rm ext} = 0$ is in good agreement with the experimental result ($T_c = 1.18$ K). This is because the gap equation is reduced to that of the BCS theory, and because the value of V_0 used in the present calculation is determined by using the critical temperature formula obtained by the BCS theory.

Next, we consider the characteristic dependence of the superconducting gap on the temperature (Fig. 3). For low magnetic fields ($B_{\rm ext} \leqslant 45$ G) of Fig. 3, $\Gamma_0(B_{\rm ext}, T)$ remains almost constant with increasing temperature, and rapidly decreases near the critical temperature. This temperature dependence is similar to the zero-magnetic-field case. The temperature dependence of $\Gamma_0(B_{\rm ext}, T)$ for high magnetic fields ($B_{\rm ext} > 45$ G) is different from that for the low magnetic fields. That is, the superconducting gap slightly increases with temperature, and then rapidly decreases near the critical

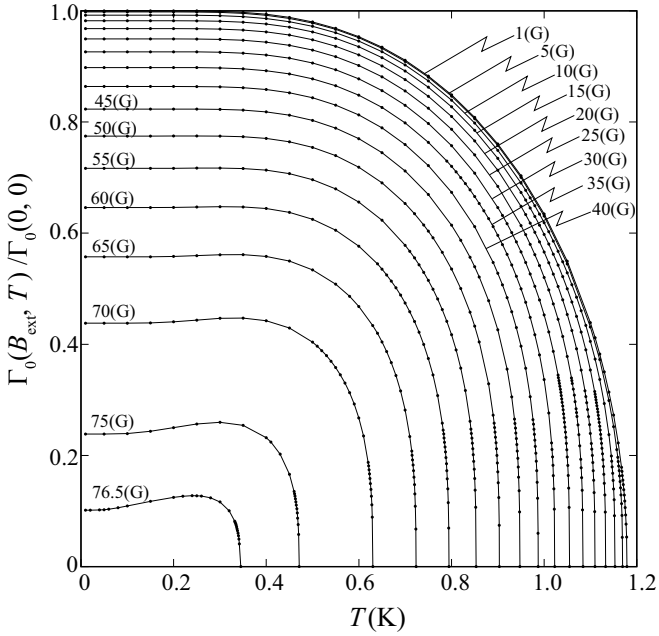

FIG. 3. Temperature dependence of the superconducting gap for fixed magnetic fields.

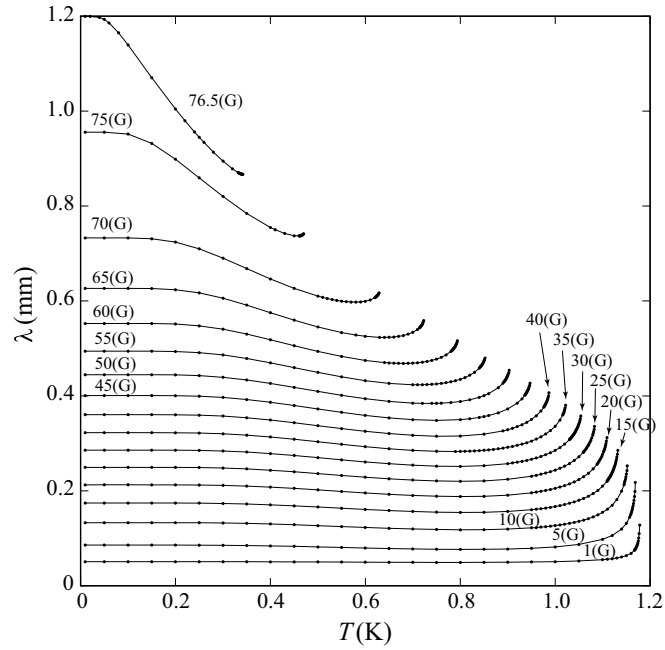

FIG. 5. Temperature dependence of the number of superconducting electrons for fixed magnetic fields.

temperature. This characteristic dependence of $\Gamma_0(B_{\text{ext}}, T)$ on temperature is revealed only after solving the gap equation for superconductors immersed in a magnetic field.

To understand the characteristic dependence, the temperature dependence of the total number of superconducting electrons $2n^{(2)}_{\text{max}}(B_{\text{ext}}, T)$ is calculated. As shown in Fig. 4, $2n^{(2)}_{\text{max}}(B_{\text{ext}}, T)$ decreases gradually with temperature, and rapidly decreases near the critical temperature. Considering that the required number of electrons contributing to the diamagnetic current of the Meissner effect is determined by the strength of the magnetic field, the diamagnetic current is maintained with an increasing temperature as follows. (A) Increasing λ to increase the number of superconducting electrons that contribute to the diamagnetic current, (B) increasing the density of superconducting electrons near the surface, or (C) increasing the velocity of superconducting electrons near the surface. In the case of (C), the kinetic energy increases, so case (C) cannot be realized. The increase of λ [case (A)] would lead to the decrease of the diamagnetic potential energy, while it leads to the decrease of the superconducting gap which causes the reduction of the superconducting energy gain. Figure 5 shows the temperature dependence of λ. The value of λ decreases with an increasing temperature, and then upturns near the critical temperature. This means that case (A) is realized near the critical temperature. In the other temperature range, case (B) seems to be realized with decrease in λ. This is because, according to the London theory, λ is inversely proportional to the square root of the superconducting electron density. Therefore, the temperature dependence of λ (Fig. 5) suggests that the density of superconducting electrons near the surface increases with temperature; therefore, λ decreases with an increasing temperature. Thus, we may say that case (B) is realized with a decrease in λ. The rate of decrease of λ becomes larger at a higher magnetic field, as shown in Fig. 5. This would be because the required number of electrons contributing to the diamagnetic current of the Meissner effect becomes larger at a higher magnetic field, so that the density of the superconducting electron becomes larger near the surface [case (B)]. Due to this decrease of λ, the superconducting gap increases with temperature (at low T) for high magnetic fields (Fig. 3). Thus, the characteristic dependences of both the superconducting gap and penetration depth on temperature are strongly related to the Meissner effect.

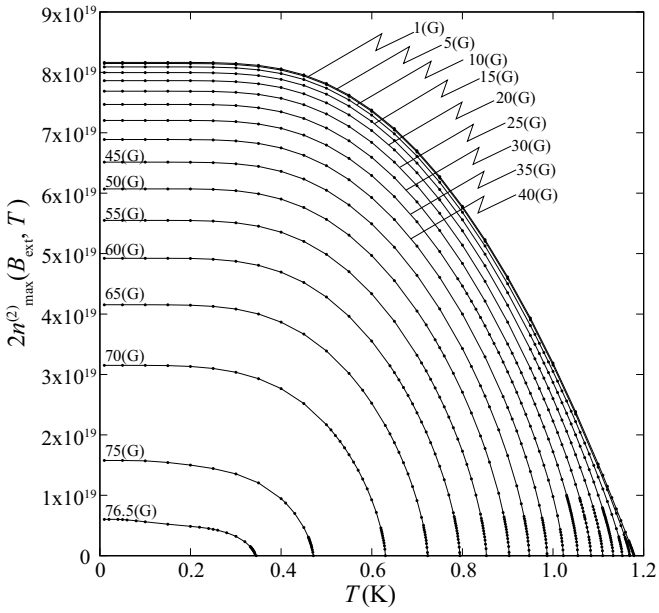

FIG. 4. Temperature dependence of the penetration depth for fixed magnetic fields.

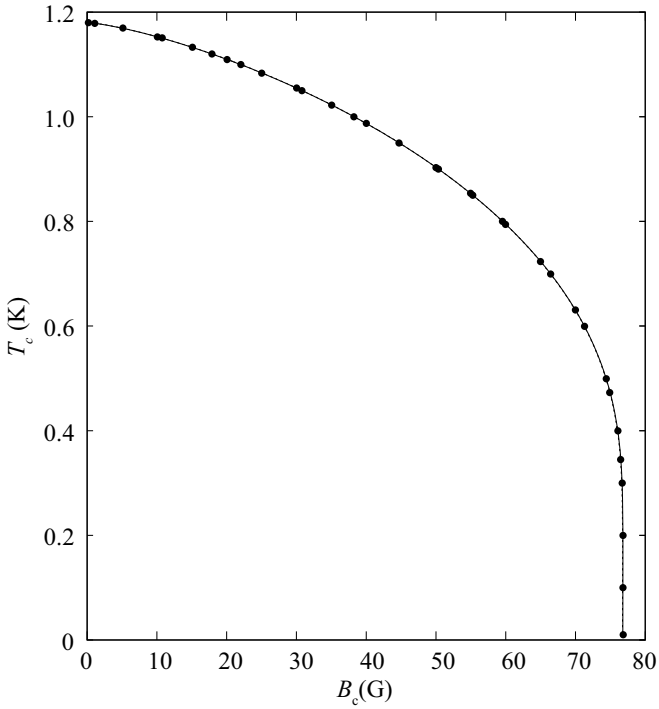

FIG. 6. Relation between the critical temperature and critical magnetic field.

Finally, the cross section of Fig. 1 at the $\Gamma_0(B_{\rm ext}, T) = 0$ plane is shown in Fig. 6. The curve in Fig. 6 indicates the phase boundary between the superconducting and normal phases. The superconducting state is stable in the inner region of the curve, where the superconducting gap has a finite value. The temperature dependence of the critical magnetic field is qualitatively consistent with experiments.

Thus, the present scheme was successfully applied to superconductors immersed in a magnetic field, and it can predict the temperature and magnetic properties of the superconducting gap.

V. CONCLUSION

This paper presents a gap equation for superconductors immersed in a magnetic field, based on a first-principles calculation method, i.e., CDFT for superconductors. This gap equation enables us to describe the magnetic and temperature behaviors of the gap for superconductors immersed in a magnetic field. Furthermore, we present a calculation scheme to solve the gap equation in consistency with a proposed relation for the superconducting energy gain for superconducting electrons. The presented scheme is applicable to superconductors immersed in a magnetic field and can predict both the temperature dependence and magnetic-field dependence of the superconducting gap.

The proposed scheme was applied to aluminum immersed in a magnetic field; it predicted the characteristic dependence of the superconducting gap on the magnetic field. In addition, the resultant critical temperature and magnetic field were in good agreement with those obtained experimentally. These calculation results demonstrate the usefulness and validity of the presented scheme.

In the derivation of the gap equation, the attractive interaction part of the exchange-correlation energy functional was evaluated within the mean-field approximation. If the approximate form is improved beyond the mean-field approximation, a gap equation similar to Eqs. (38) or (40) would be obtained. Furthermore, if the approximate form for the exchange-correlation energy functional that induces the OPSS with spin-triplet symmetry [27] is employed, the gap equation for superconductors with triplet OPSS can be developed in a similar manner to the presented gap equation. Thus, the proposed scheme has extensive utility and provides a useful framework for describing the properties of superconductors immersed in a magnetic field.

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