Determinations of upper critical field in continuous Ginzburg-Landau model

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Novel procedures to determine the upper critical field $B_{c2}$ have been proposed within a continuous Ginzburg-Landau model. Unlike conventional methods, where $B_{c2}$ is obtained through the determination of the smallest eigenvalue of an appropriate eigen equation, the square of the magnetic field is treated as eigenvalue problems so that the upper critical field can be directly deduced. The calculated $B_{c2}$ from the two procedures are consistent with each other and in reasonably good agreement with existing theories and experiments. The profile of the order parameter associated with $B_{c2}$ is found to be Gaussian-like, further validating the methodology proposed. The convergences of the two procedures are also studied.

I. INTRODUCTION

The determinations of the upper critical field $B_{c2}$ are based on the Ginzburg-Landau-Abrikosov-Gorkov (GLAG) framework that is applicable to practically all superconductors. The starting point of the macroscopic description is the first Ginzburg-Landau (GL) equation or its similarities. Examples would be the standard linearized GL equation, the harmonic oscillator equation, the Mathieu equation, the continuous Ginzburg-Landau equation, the GLd equation, the Ginzburg-Pitaevskii equation.

On the other hand, the linear gap equation is adopted to microscopically determine the upper critical field. This equation can be converted into an equation including the digamma function. The parameter of the digamma function is related to the smallest eigenvalue of an eigen equation with appropriate boundary conditions. Having obtained the smallest eigenvalue of the eigen equation, $B_{c2}$ may then be implicitly determined from the equation including the digamma function ($B_{c2}$ is in connection with the smallest eigenvalue). Such a procedure or its extensions may be seen, for example, in the calculations of $B_{c2}$ for type-II superconductors (s-wave), heavy-fermion superconductors (p-wave), high $T_c$ superconductors (d-wave), layered superconductors, thin films, multilayers, and organic superconductors.

It is tempting to conclude that almost all the efforts made to obtain $B_{c2}$ are via the determination of the smallest eigenvalue of an appropriate eigen equation. For instance, in Ref. 1, $B_{c2}$ is inversely proportional to the smallest eigenvalue (the lowest Landau level) of the harmonic oscillator equation.

Nevertheless, for all the GL-like equations as well as the linear gap equation, one may have a universal definition for the upper critical field: it is the maximum magnetic field at which the corresponding equation has a nontrivial solution. Such a nontrivial solution would naturally correspond to the eigen function associated with the smallest eigenvalue and would correspond to the solution to the linear gap equation at $B_{c2}$. It is worth noting that the eigen function associated with the smallest eigenvalue may be just one of the solutions to the linear gap equation (see, for example, Refs. 17,21 and 35).

Several approaches, for example, the perturbation method, and the variational technique, have been adopted to find $B_{c2}$ by obtaining the smallest eigenvalue. We note that in Ref. 1, the authors iteratively calculated the upper critical field of a thin-film superconductor with a ferromagnetic dot: first guessing a value for the upper critical field, then solving the standard linearized GL equation to make sure the calculated value of the upper critical field is equal to the guessed one. Otherwise, equate the newly calculated value to the guessed one and resolve the linear equation until the two values are equal to each other. It can be seen that such an iterative method is still related to obtaining the smallest eigenvalue.

In this paper, instead of obtaining the smallest eigenvalue, from which $B_{c2}$ is implicitly or indirectly determined, we will directly calculate $B_{c2}$: the square of the magnetic field $B^2$ is treated as an eigenvalue of an eigen equation so that $B_{c2}$ can be directly deduced from the largest eigenvalue of the eigen equation. Within a continuous Ginzburg-Landau model, two procedures will be presented to obtain the corresponding eigen equations, either of which can determine $B_{c2}$. Note that the applications of these procedures have been published in Refs. 37 and 38.

II. MODEL

The continuous Ginzburg-Landau model (CGL) is applicable to layered superconductors. The unit cell describing the layering structure consists of alternating superconducting (S) and insulating (I) layers. The $z$ axis is normal to the layers and its origin is at the midpoint of one of the I layers. The center of the S layer is located at $D/2$, where $D$ is the size of the unit cell. The GL coefficients and the effective superpair masses (perpen-
so that the vector potential can be taken as $\vec{A}$ in the free energy of Eq. 1, we get

$$F = \int d\vec{r} \int dz \left[ \alpha(T, z)|\Psi(\vec{r}, z)|^2 + \frac{1}{2} \beta|\Psi(\vec{r}, z)|^4 + \frac{\hbar^2}{2M(z)} \left( \frac{\partial}{\partial z} - \frac{2ie}{\hbar} A_z(\vec{r}, z) \right)\Psi(\vec{r}, z) \right]^2$$

$$+ \frac{\hbar^2}{2m(z)} \left( \nabla(2) - \frac{2ie}{\hbar} \vec{A}^{(2)}(\vec{r}, z) \right)\Psi(\vec{r}, z) \right|^2 + \frac{1}{2\mu_0} B^2(\vec{r}, z),$$

(1)

where $T$ is the temperature, $\vec{r} = (x, y)$ is the planar vector and $\vec{A}^{(2)}(\vec{r}, z) = (\vec{A}^{(2)}(\vec{r}, z), A_z(\vec{r}, z))$ is the vector potential. The effective masses and the GL condensation coefficient $\alpha(T, z)$ are assumed to be periodic with a period $D$. $\beta$, however, is held fixed as it does not affect the qualitative behavior of the studied system. As before, we choose

$$\alpha(T, z) = [\alpha_0 + \alpha_1 \cos(2\pi z/D)](1 - T/T_c),$$

(2a)

$$\frac{1}{M(z)} = G_0 + G_1 \cos(2\pi z/D),$$

(2b)

$$\frac{1}{m(z)} = g_0 + g_1 \cos(2\pi z/D),$$

(2c)

where $T_c$ is the transition temperature. $\alpha_0, \alpha_1, G_0, G_1, g_0$ and $g_1$ are model parameters. Note that for dirty materials, the linear GL theory for $B_{c2}$ may be extended to low temperatures.

Let an external field $B$ be applied along the $y$-direction so that the vector potential can be taken as $\vec{A} = (Bz, 0, 0)$. Assuming $\Psi(\vec{r}, z) = e^{i\vec{k} \cdot \vec{r}} \Psi(z)$ and minimizing the free energy of Eq. 1, we get

$$-\frac{\hbar^2}{2M(z)} \frac{\partial^2}{\partial z^2} \Psi(z) - \frac{\hbar^2}{2} \left[ \frac{\partial}{\partial z} \frac{1}{M(z)} \right] \frac{\partial}{\partial z} \Psi(z) +$$

$$\left[ \frac{1}{2m(z)}(2eB)^2(z - z_n)^2 + \frac{\hbar^2 k^2}{2m(z)} \right] \Psi(z) +$$

$$\alpha(T, z) \Psi(z) + \beta|\Psi(z)|^2 \Psi(z) = 0,$$

(3)

with $z_n = \hbar k_z/(2eB)$. At $B = B_{c2}$, the order parameter is small enough so that the term $\beta|\Psi(z)|^2 \Psi(z)$ in Eq. 3 can be omitted. The superconducting order at $B_{c2}$ nucleates in the S layer first so that one may choose $z_n = D/2$. To explore the features of the order parameter along the $z$-direction, one may assume $k_y = 0$. Finally, we arrive at the following equation,

$$-\frac{\hbar^2}{2M(z)} \frac{\partial^2}{\partial z^2} \Psi(z) - \frac{\hbar^2}{2} \left[ \frac{\partial}{\partial z} \frac{1}{M(z)} \right] \frac{\partial}{\partial z} \Psi(z) +$$

$$\left[ \alpha(T, z) + \frac{1}{2m(z)}(2eB)^2(z - D/2)^2 \right] \Psi(z) = 0.$$

(4)

At a given temperature $T$, the maximum magnetic field $B$ at which a nontrivial solution satisfies the above equation gives a point in the $B_{c2}$-$T$ plot. Eq. 4 will be numerically solved subject to the following boundary conditions,

$$\Psi(0) = \Psi(D),$$

(5a)

$$\frac{\partial}{\partial z} \Psi(z) \bigg|_{z=D} = 0.$$

(5b)

Note that neglecting the size effect in the $z$-direction and considering the layering structure and the superposition of different superpairs as a mean field effect, the variation of the macroscopic wave function—the order parameter along the $z$-direction may have a periodic property (for example, see Ref. [11]). It should be mentioned that the new methodology of determining the upper critical field, which is to be described below, is also applicable to other boundary conditions.

III. METHODOLOGY

A. Procedure I

Taking into account the boundary conditions of Eq. 5, Eq. 4 can be transformed into a system of equations which can be simplified to

$$U\Psi = 0,$$

(6)

where $\Psi = (\Psi_1, \Psi_2, ..., \Psi_{2n+1})'$ is a column vector representing the discrete solutions of Eq. 4. The symbol $'$ here indicates transpose and $n$ is a positive integer. $U$ is a $(2n+1) \times (2n+1)$ sparse matrix having the following structure.
where \(A_i, B_i, C_i, D_i\) and \(E_i\) are the coefficients of the discretized equations of Eq. 4. In the first row of \(U\), the boundary condition \(\Psi(0) = \Psi(D)\) (Eq. 5) is explicitly written as \(\Psi_1 = \Psi_{2n+1}\) while in the last row, the discretization of \(\left. \frac{\partial}{\partial z} \Psi(z) \right|_{z=D} = 0\) (Eq. 6) is implemented as \(-2\Psi_2 - \Psi_{2n-1} + 6\Psi_{2n} - 3\Psi_{2n+1} = 0\). The periodic property of the solutions is taken into consideration in the last row (\(\Psi_{2n+2} = \Psi_2\)), in the second row (see \(A_2\)) and in the second last row (see \(E_{2n}\)).

It is easy to verify that only the \(C_i\) coefficients contain the magnetic field \(B\) and these coefficients can be separated into two terms, where one of them is \(B\)-dependent:

\[
C_i = C_i^0 + C_i^B \cdot B^2. \tag{8}
\]

To obtain \(B_{c2}\) with our method, we require that there be no prefactor appearing before the square of the magnetic field \(B^2\). Hence, the factor \(C_i^B\) in Eq. 8 should be divided. To cure the division singularity at \(z = D/2\) (i.e., \(C_i^B = 0\) at \(i = n + 1\) in Eq. 8), a solution property \(\left. \frac{\partial}{\partial z} \Psi(z) \right|_{z=D/2} = 0\) is assumed and implemented in the middle row of \(U\) as

\[ -2\Psi_1 - 3\Psi_{n+1} + 6\Psi_{n+2} - \Psi_{n+3} = 0 \] (different from the approximation in the last row).

For Eq. 8 to have non-trivial solutions, the determinant of \(U\) should be zero,

\[
\det[U] = 0. \tag{9}
\]

By eliminating the constant elements in the first, middle and last rows of \(U\) and separating \(C_i\) into the two terms with the negative prefactor \(-C_i^B\) excluded (cf. Eq. 8), \(\det[U]\) can be transformed into

\[
\det[P - B^2 I] = 0, \tag{10}
\]

where \(I\) is a unitary matrix and \(P\) is a matrix without the magnetic field (see below). Thus, the largest solution for \(B\), namely \(B_{c2}\), can be easily available just by obtaining the largest positive eigenvalue of the eigen equation,

\[
P = B^2 \Phi, \tag{11}
\]

where \(\Phi\) is the eigen function and \(P\), with the dimension of \((2n - 2) \times (2n - 2)\), has the following structure,
where $A'_i = -A_i/C^B_i$, $B'_i = -B_i/C^B_i$, $C^0_i = -C^0_i/C^B_i$, $D'_i = -D_i/C^B_i$ and $E'_i = -E_i/C^B_i$. Here, $i \neq n + 1$ and thus the division singularity is avoided. Having determined $B_{c2}$ from Eq. 11, one can obtain the corresponding order parameter by substituting $B_{c2}$ back into Eq. 10.

### B. Procedure II

In the above procedure, the upper critical field is obtained by treating the square of the magnetic field $B^2$ as an eigenvalue (Eq. 11). Following the same idea, one may obtain a straightforward procedure from Eq. 11

$$Q \Psi = B^2 \Psi,$$

where $\Psi = (\Psi_1, \Psi_2, ..., \Psi_{2n})'$, which has the same meaning as that in Eq. 10. However, to avoid the singularity at $z = D/2$, the dimension of the current $\Psi$, $2n$, is set different from the previous one, $2n + 1$. The matrix $Q$ has the following structure:

$$
\begin{pmatrix}
C^0_1 & D_1 & E_1 \\
B_2 & C^0_2 & D_2 & E_2 \\
A_3 & B_3 & C^0_3 & D_3 & E_3 \\
A_4 & B_4 & C^0_4 & D_4 & E_4 \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
A_{2n-3} & B_{2n-3} & C^0_{2n-3} & D_{2n-3} & E_{2n-3} \\
A_{2n-2} & B_{2n-2} & C^0_{2n-2} & D_{2n-2} & E_{2n-2} \\
E_{2n-1} & & & & \\
D_{2n} & E_{2n} \\
\end{pmatrix}

\begin{pmatrix}
A_1 & B_1 \\
A_2 & \end{pmatrix}

\right) \right)

The dimension of $Q$ is $2n \times 2n$, larger than that of $P$ but smaller than that of $U$. 

Eq. 13 implies that one may directly determine the upper critical field from the linear GL equation. The
IV. RESULTS AND DISCUSSION

Bi2212 has been chosen as our modeling prototype since it possesses a large anisotropy, and is thus suitable for studies of properties related to the layered structure. The values of the parameters for Bi2212 are taken from Ref. 37. The calculated $B_{c2}$ at zero temperature for various $n$ are shown in Table I. It can be seen that the two sets of data calculated from Eqs. 11 and 13 converge finally and the convergent values are in good agreement with each other.

A glance at the data for $B_{c2}$ in Table I shows that Procedure II converges more rapidly than Procedure I. Hence, using $B_{c2}(n = 1200)$ from Procedure II for the convergence analysis, the error is defined as

$$E_n = |B_{c2}(n) - B_{c2}(n = 1200)|.$$

This equation is applicable to both procedures and the corresponding errors are listed in Table I and plotted in Fig. 1. It is found that the errors of the two procedures can be respectively fitted as

$$E_n = \begin{cases} E_{n_0}(n_0/n)^3 \propto n^3 & \text{for Procedure I}, \\ E_{n_0}(n_0/n)^4 \propto n^4 & \text{for Procedure II}. \end{cases}$$

TABLE I: Values of $B_{c2}$ (SI unit) for various $n$, treated as eigenvalue problems from different procedures. The error is $E_n = |B_{c2}(n) - B_{c2}(n = 1200)|$, where $B_{c2}(n = 1200) = 3338.680126$ Tesla.

| Eigen equation | $n$  | $B_{c2}$       | $E_n$  |
|----------------|-----|----------------|-------|
|                | 50  | 3265.749101    | 72.93 |
|                | 100 | 3328.453273    | 10.23 |
| Eq. II (Procedure I) | 200 | 3337.366920     | 1.314 |
|                | 400 | 3338.513958    | 0.1662|
|                | 800 | 3338.658438    | 0.02169|
|                | 50  | 3339.154981    | 0.4749 |
|                | 100 | 3338.709744    | 0.02962|
| Eq. III (Procedure II) | 200 | 3338.681966     | 0.001840|
|                | 400 | 3338.680240    | 1.135E-4|
|                | 800 | 3338.680132    | 6.020E-6|

Here $n_0$ is taken to be 50 and $E_{n_0}$ is the corresponding error. The grid spacing $h \sim D/2n$, when $n$ is large. From these fits, we know that the error of Procedure I is of order 3 while that of Procedure II is 4, which are consistent with the error orders of the approximations used in the matrices $U$ and $Q$, respectively.

Note that $B_{c2}$ at 0 K in the tables may be comparable to those extrapolated (using the WHH theory) from some experiments (for example, see Ref. 43). By choosing appropriate values of the model parameters, the extrapolated result of 2640 Tesla for Bi2212 can be obtained exactly.

We find that the order parameters obtained from Eqs. (10) and (13) are also consistent with each other. In the following calculations, Procedure II is employed. In Fig. 2, we plot the spatial distribution of the calculated order parameter at $T/T_c = 0.9$. It is found that for Bi2212 in a large temperature range, the asymptotic behavior of the order parameter can be expressed as

$$\Psi(z) \sim C \exp \left[ -\frac{(z - D/2)^2}{2\xi^2} \right],$$

which is exactly the ground state of the linearized GL equation at $B_{c2}$. The Gaussian profile of the order parameter is also similar to the shape of the pair amplitude in bulk superconductors. In fact, it is natural that the order parameter of the largest eigenvalue of $B^2$ should be just that of the lowest eigenvalue for the linear equation, due to the inverse relation between $B$ and the eigenvalues of the linear equation.

When near $T_c$ or in a less anisotropic superconductor such as YBCO, we found that an offset of the Gaussian...
FIG. 2: Spatial distribution of the order parameter at $T/T_c = 0.9$, which can be approximated by the well-known Gaussian function.

order parameter (Eq. 17) can not be neglected. Hence, one may infer that the mean field effect or the interlayer coupling of the order parameter has less influence on a highly anisotropic superconductor at low temperatures (2-D feature) than on a superconductor at high temperatures or with a small anisotropy.

The finding here that a Gaussian-like exponential component contributes to the order parameter may adequately signify that the eigen function associated with the maximum magnetic field eigenvalue of the linear GL equation is equivalent, to a certain extent, to the eigen function related to the lowest eigenvalue of the linear GL equation. The latter eigen function may have the form $\exp \left[ \frac{Bc^2}{\Phi_0} (z - D/2)^2 \right]$ (cf. Eq. 4.73 in Ref. 5). Comparing this function to the Gaussian-like exponential contribution (Eq. 17), one has $Bc^2 \propto 1/\xi^2$. For Bi2212, we find that $1/\xi^2 \propto 1 - T/T_c$ is satisfied for a large temperature range (Fig. 4), hence, $Bc^2 \propto 1 - T/T_c$ (see Fig. 4). Similarly, we also have found that the linear $Bc^2 - T$ relation is satisfied in YBCO. Such a linear feature is consistent with the general $Bc^2 - T$ picture in layered cuprates near $T = 0$ K, and is in agreement with the anisotropic GL theory and some other theories. Experimentally, the linear behavior away from $T_c$ was observed in YBCO.

FIG. 3: Linear relation between $1/\xi^2$ and $1 - T/T_c$, where $\xi$ is the parameter characterizing the width of the Gaussian order parameter.

A closer inspection of Fig. 4 reveals that near $T_c$, the $Bc^2 - T$ plot exhibits a square-root-like behavior which is in agreement with Feinberg’s theory. This behavior is also found in twinned superconductors, multilayers, and thin films. In one of the earliest papers, Ginzburg and Landau correctly predicted that $Bc^2$ for thin films varied as $\sqrt{\phi - T}$ when $T \rightarrow T_c$, as a consequence of the boundary conditions. This was subsequently confirmed experimentally by Khukhareva.

In our calculations, we found that near $T_c$, the height of the Gauss component $C$ in Eq. 17 decreases with temperature and hence, the order parameter is nearly constant (3-D feature). Qualitatively speaking, the nearly constant order parameter near $T_c$ for the layered superconductors is equivalent to the case of thin films so that one can observe the square-root behavior near $T_c$. In fact, the boundary condition of Eq. 5b applies only to thin films. More precisely, with a constant solution to the order parameter, one can immediately infer from Eq. 5b that there exists a square-root relationship between $Bc^2$ and $1 - T/T_c$. It is worth noting that Dediu et al. also obtained a square-root $Bc^2 - T$ relation near $T_c$ by solving the usual GL equations and the feature of the order parameter near $T_c$ was used to interpret their results.

It is interesting to note that in the $Bc^2 - T$ plot, the transition from square-root to linearity may be consid-
V. CONCLUSION

The conventional work to determine upper critical fields should resort to obtaining the smallest eigenvalue of an appropriate eigen equation. However, within a continuous Ginzburg-Landau model, we have demonstrated through two procedures that one can obtain the upper critical field by treating the square of the magnetic field as an eigenvalue problems, from which $B_{c2}$ can be directly deduced.

The calculated $B_{c2}$ from the two procedures are consistent with each other and in reasonably good agreement with existing theories and experiments. The profile of the order parameter obtained at $B_{c2}$ is Gaussian-like, further indicating the plausibility of the procedures proposed.

The convergences of the proposed procedures were also investigated to identify the efficiency of the procedures. It was found that the more direct method, Procedure II, converges faster than Procedure I. The corresponding convergent error orders of the two procedures are 4 and 3, respectively. These orders are consistent with the orders of the approximations used in our calculations.

Note that certain physical phenomena such as fluctuations and spin-orbit scattering may have some influences on the upper critical field. The present procedures proposed may serve as a starting point to further study more properties of upper critical fields.

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