Theory of Upper Critical Field without Energy Quantization

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Conventional theories for determining upper critical fields are inevitably related to the lowest eigenvalues of appropriate equations. In this Letter, a new theory of upper critical fields is designed and justified. Using MgB$_2$ as modeling prototype, our computations are in excellent agreement with the Ginzburg-Landau theory. The long-standing issue, the upward curvature of the upper critical field, is found to be a manifestation of the crossover of the order parameter. The current theory is an alternative to the traditional technique of energy quantization in determining upper critical fields.

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The upper critical field ($B_{c2}$) is the maximum magnetic field that a bulk type-II superconductor can sustain in the superconducting state. The value of $B_{c2}$ is very important as it partially determines the current carrying capacity of the superconductor and its uses e.g. to produce high field superconducting magnets. Furthermore, study of properties of $B_{c2}$ may test the validity of various theoretical models and provide information for important superconducting parameters such as the coherence length. Hence, research of the upper critical field is of practical, fundamental and enduring interest.

To determine the upper critical field, an important starting point is the linearized Ginzburg-Landau (GL) equation and its variants. Examples would be the quantum harmonic oscillator equation, the Mathieu equation, the $p$-wave GL equation, and the $d$-wave GL equation. Determining upper critical fields from these equations involves finding the lowest eigenvalues of the said equations. Alternatively, the microscopic description of the upper critical field, based on the Gor'kov gap equation, may also be reduced to finding the lowest eigenvalues of appropriate equations. Note that the eigenstate of the lowest eigenvalue of the linearized GL equation is usually chosen as the trial function in the variational determinations of $B_{c2}$ (see, e.g., Refs. [6] [11]). Thus, the variational treatment is related to the lowest-eigenvalue method. Note further that the perturbation approach to determining upper critical fields is also intimately related to the scenario of the lowest eigenvalue. Consequently, we are led to conclude that almost all the efforts [1, 2, 3, 4, 7, 8, 9, 10, 11, 12] for determining upper critical fields are related to the lowest eigenvalue of an appropriate equation, which is in turn, more or less, explicitly or implicitly, related to the important concept of energy quantization [1, 2, 13, 14]. This traditional framework of determining upper critical fields by energy-quantization related techniques or scenarios has existed for fifty years or so [1, 2, 3]. However, in this Letter, a new theory will be reported and justified to determine upper critical fields without recourse to energy quantization. Some applications and implications of the theory proposed will also be addressed.

Various superconductors are layered compounds although they may be oxides, metallic or organic. To describe layered superconductors, a continuous Ginzburg-Landau (CGL) model was proposed [10], in which the GL coefficients and the superpair masses are assumed spatially dependent. This model was considered [10] to approach the limiting cases of the anisotropic Ginzburg-Landau (AGL) theory (see Ref. [15] and references therein) and the Lawrence-Doniach (LD) model [16].

Recently, a modified CGL model has been proposed [17, 19, 20]. The unit cell in this model consists of alternating superconducting and weakly superconducting layers. The $z$-axis is normal to the layers and its origin is at the midpoint of one of the weakly superconducting layers. The center of the superconducting layer is located at $D/2$, where $D$ is the size of the unit cell [19, 20]. Applying an external magnetic field $B$ parallel to the layers, the linearized CGL equation may be written as [10, 13, 19, 20, 21]

\[
- \frac{\hbar^2}{2M(z)} \frac{\partial^2}{\partial z^2} \Psi(z) - \frac{\hbar^2}{2} \left[ \frac{\partial}{\partial z} \frac{1}{M(z)} \frac{\partial}{\partial z} \right] \Psi(z) + \left[ \alpha(T, z) + \frac{1}{2m(z)} (2eB)^2 \left( z - \frac{D}{2} \right)^2 \right] \Psi(z) = 0, \tag{1}
\]

where the nucleation center ($z_c = \hbar k_z/2eB$) is set at $D/2$. The condensation coefficient $\alpha(T, z)$ and the effective masses, $M(z)$ and $m(z)$, are assumed as [10, 20, 21]

\[
\alpha(T, z) = |a_0 + a_1 \cos(2\pi z/D)| (1 - T/T_c), \tag{2a}
\]

\[
\frac{1}{M(z)} = G_0 + G_1 \cos(2\pi z/D), \tag{2b}
\]

\[
\frac{1}{m(z)} = g_0 + g_1 \cos(2\pi z/D). \tag{2c}
\]

Here $a_0$, $a_1$, $G_0$, $G_1$, $g_0$ and $g_1$ are model parameters and the determinations of their values can be found in Ref. [20].

To determine the upper critical field, Eq. (1) should be completed by appropriate boundary conditions. Here we
choose the open boundary conditions (OBCs),
\[ \Psi(z)|_{z \to \pm \infty} = 0. \]  

Eq. (3) and (6) can be transformed into a system of the form
\[ U\Psi = 0, \]
where \( \Psi \) is a wave function representing the discrete solutions of Eq. (1) and \( U \) is the corresponding coefficient matrix \[22\]. For Eq. (1) to have non-trivial solutions, the determinant of \( U \) should be zero,
\[ \det[U] = 0. \]

It can be verified \[22\] that the parameters of the magnetic field \( B \) appear only in the main diagonal of \( U \) so that we have
\[ \det[P - B^2 I] = 0, \]
where \( I \) is a unitary matrix and \( P \) is a sparse matrix independent of \( B \). Thus, the maximum \( B \), namely the upper critical field, can be deduced from the largest eigenvalue of the following eigen equation
\[ P\chi = B^2\chi, \]
where \( \chi \) is the eigenfunction of \( P \) and this function is an auxiliary field to Eq. (1). Having determined \( B_{c2} \), one can obtain the corresponding order parameter by substituting \( B_{c2} \) back into Eq. (1).

It should be stressed that Eq. (1) can be written as
\[ \hat{Q}\Psi(z) = B^2\Psi(z), \]
where \( \hat{Q} \) is an operator. Eq. (3), together with the boundary conditions of Eq. (1), can be written as the following matrix eigen equation \[22\],
\[ Q\Psi = B^2\Psi, \]
where \( \Psi \) possesses the same meaning as in Eq. (1). \( Q \) is the same as \( P \) in Eq. (7). Hence, Eq. (9) is equivalent to Eq. (7) and \( \Psi \) plays the same role as \( \chi \) as eigenfunctions.

For comparison of our determinations with the traditional treatment for bulk superconductors \[1, 2, 23, 24\], we model the MgB\(_2\) superconductor \[25\] whose anisotropy is small \[22, 26\]. For convenience, we treat it to be isotropic and ignore the spatial dependences in Eq. (2). Hence, \( G_0 = g_0 = 1/m = 0.5 \) and \( G_1 = g_1 = \alpha_1 = 0 \) were chosen and the nucleation center set at \( z_c = 0 \). Other parameters such as \( \alpha_0 \) for MgB\(_2\) are taken from Ref. \[20\]. It was found that (see Fig. 1) the results obtained from Eq. (9) are strikingly in agreement with the traditional GL work \[1, 2, 23, 24\],
\[ B_{c2} = \Phi_0/2\pi \xi^2 = \sqrt{\kappa} B_c, \]
where the flux quantum \( \Phi_0 = h/2e \) and the coherence length \( \xi = \sqrt{2m|\alpha(T)|} = \sqrt{2} \alpha_0/(1 - T/T_c)/\hbar \). \( B_c \) is the thermal dynamic critical field and \( \kappa \) is the ratio of the penetration depth \( \lambda \) to the coherence length \( \xi \). It should be emphasized that Eq. (10) is derived from energy quantization of the quantum harmonic oscillator equation \[1, 2, 22\] and the microscopic theory \[6\] may also arrive at a similar expression. The agreement of our calculations with Eq. (10) lends us strong credence to our theory of upper critical fields. Furthermore, we found that the calculated results are reasonably consistent with the experiments of Finnemore et al. \[26\] and with some theoretical results \[22, 27\], as shown in Fig. 1. These agreement and consistencies show that MgB\(_2\) is a superconductor describable within the GL/BCS framework. Note, however, that our main interest here lies in the qualitative predictions of the theories and thus we have assumed that the theories arrive at the same value of \( B_{c2} \) at zero temperature; otherwise, the actual values are deviated from the zero-temperature one but the qualitative trends remained.

In Fig. 2 we have plotted the spatial distribution of the order parameter at \( B_{c2} \), which was obtained from Eq. (7) at \( T = T_c/2 \). It can be seen that the order parameter is in excellent agreement with the following function at \( n = 0 \) (in a.u.)
\[ \Psi_n(z) = \frac{1}{\pi^{1/4}\xi^{1/2}\sqrt{2^n n!}} \exp\left(-\frac{z^2}{2\xi^2}\right) H_n\left(\frac{z}{\xi}\right), \]
where \( \xi = 1/\sqrt{2B_c} \) and \( H_n \) are Hermite polynomials. Eq. (11) represents the eigenstates of the harmonic oscil-
FIG. 2: Order parameters at the upper critical field, the second and third largest square of the magnetic field respectively correspond to the ground, first and second excited states of the quantum harmonic oscillator [Eq. (11)].

The function at \( n = 0 \) is the state of the lowest energy eigenvalue. The remarkable agreements of our calculations with Eqs. (10) and (11) unambiguously justifies the current theory of upper critical fields.

It is interesting to find that (see Fig. 2) the order parameters corresponding to the second and third largest \( B^2 \) are nothing else but the first and second excited states of the harmonic oscillator equation, as given by Eq. (11) at \( n = 1, 2 \), respectively. Note that in the expression of \( \zeta = 1/\sqrt{2B_c^2} \), \( B_c^2 \) should now be replaced by \( B_2^2 \) and \( B_3^2 \), which are the square roots of the second and third largest \( B^2 \), respectively. Here, a few points are worthy of notice.

(i) What does \( B \) associated with the lowest eigenvalue of \( B^2 \) mean? Which state are superconductors in subject to such \( B \)? The respective possible answers might be the lower critical field and the Meissner state? (ii) Are there any physical consequences in Eq. (9) or Eq. (7) by changing \( 2e \) to \( e \) in Eq. (1)? Are there any other physical significances in Eqs. (7) and (9) themselves except being used to obtain upper critical fields? (iii) The sign of \( \alpha_0 \) in Eq. (2a) may need attention: by setting positive condensation energy \( \alpha_0 \) (with \( \alpha_1 = 0 \)), it was found that the calculated upper critical field is always zero. Hence, negative condensation energy is a necessity for a superconducting state, as expected.

Now some applications and implications of our theory will be addressed. The upward (positive) curvature of the \( B_{c2}-T \) curve in layered superconducting systems is a subject of long-term interest. A linear behavior also holds at low temperatures \([21, 22]\). Hence, a transition exists linking the two kinds of linear behaviors. In Fig. 3(b), the spatial distributions of the corresponding order parameters are presented, where \( \Delta t = 0.0004 \) was chosen for clarity. It is clear that the order parameters below \( t^* \sim 0.998 \) mainly reside within one unit cell whereas for \( t > t^* \), the order parameters spread over several unit cells. This crossover of the order parameter manifests itself as the upward curvature observed in (a).

FIG. 3: Upper critical field and order parameter of Bi2212 near \( T_c \). (a) Upper critical field as a function of reduced temperature \( t = T/T_c \), showing an upward curvature at \( t^* \sim 0.998 \). (b) Spatial distributions of the order parameters near \( T_c \). For \( t < t^* \), the order parameters are mainly confined within one unit cell whereas for \( t > t^* \), the order parameters spread over several unit cells. This crossover of the order parameter manifests itself as the upward curvature observed in (a).

is clear that at \( t^* \sim 0.998 \), an upward curvature appears. In the extreme vicinity of \( T_c \), the \( B_{c2}-T \) plot is linear (which is consistent with the GL and AGL theories). A linear behavior also holds at low temperatures \([21, 22]\). Hence, a transition exists linking the two kinds of linear behaviors. In Fig. 3(b), the spatial distributions of the corresponding order parameters are presented, where \( \Delta t = 0.0004 \) was chosen for clarity. It is clear that the order parameters below \( t^* \sim 0.998 \) mainly reside within one unit cell whereas those above \( t^* \) spread into the neighboring cells. With increasing temperature, more layers are penetrated [i.e., three dimensional (3D) behavior] whereas those above \( t^* \) spread into the neighboring cells. Thus, \( t^* \) is a crossover temperature for the order parameter to transit between the 2D and 3D behaviors. Clearly, the upward curvature [Fig. 3(a)] is originated from the crossover of the order parameter [Fig. 3(b)], which is in turn due to that the layering structures [cf. Eq. (4)] come into effects. Note that the value of \( t^* \sim 0.998 \) obtained here for Bi2212 is consistent with Ref. \([37]\), in which the most likely value was estimated in the range 0.997-0.998.

It is worth mentioning that by considering the small
anisotropy in MgB$_2$ ($G_0 \sim 1$, $g_0 \sim 1$ and $G_1 = g_1 = \alpha_1 = 0$), our calculations are consistent with the AGL theory. Moreover, CGL simulations have also been performed for MgB$_2$ but no obvious upward curvature was observed. In fact, the issue of the upward feature is quite complicated \[21, 31, 32\]. A recent experimental study \[33\] shows that the upward curvature may also exist in MgB$_2$. If the same reason for the curvature, i.e., the crossover of the order parameter, is also applicable to MgB$_2$, one can expect that the influence of layered structure on MgB$_2$ should be less prominent than that on the highly anisotropic superconductor Bi2212. Note that besides the upward feature obtained, we have also achieved a square-root field temperature dependence \[20, 21\] within our framework.

The theory reported here is generic. It can be used to study various properties of upper critical fields not only in different superconductors \[20\], different boundary conditions \[21, 22\] and different dimensions \[35\], but also possibly in surface \[30\] and d-wave \[5\] superconductivity and in the Gor’kov gap equation \[4\]. Moreover, the scheme in our theory may be used to determine the transition temperature of a superconductor in a magnetic field since the relationship between the upper critical field and temperature is equivalent to that between the critical temperature and the applied field.

Our theory is an alternative to the traditional quantum-mechanical determinations of upper critical fields. The latter techniques are somehow related to the lowest eigenvalue (energy quantization) of the quantum harmonic oscillator equation. However, we have shown in this Letter that, instead of resorting to traditional method of energy quantization, the quantum harmonic oscillator equation can be treated just in a “classical” manner (i.e., directly utilize the largest eigenvalue of the square of the magnetic field) to determine upper critical fields. It is known that some fundamental enigmas of quantum theory remain unresolved \[40, 41\] and tested \[42\]. Our success tempts us to ponder more about the techniques of quantum mechanics and to ask questions such as what is the origin of the wave function (which is the central puzzle of quantum mechanics \[42\])? It is clear that the concept of energy quantization can be bypassed in the present theory of upper critical fields. Moreover, the $\Psi$ function in Eq. \[4\] is equivalent to the $\chi$ function in Eq. \[1\] while $\chi$ is an auxiliary field to Eq. \[1\]. Hence $\Psi$ is an auxiliary field? Whether quantum mechanics needs interpretations or not \[1\], the theory itself is of profound mathematical beauty \[43\] and has achieved brilliant success \[40\].

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[1] A. A. Abrikosov, Zh. Eksp. Teor. Fiz. 32, 1442 (1957) [Sov. Phys.-JETP 5, 1174 (1957)].
[2] V. L. Ginzburg and L. D. Landau, Zh. Eksp. Teor. Fiz. 20, 1064 (1950).
[3] R. A. Klemm et al., Phys. Rev. B 12, 877 (1975).
[4] J. X. Zhu et al., Phys. Rev. B 56, 14093 (1997).
[5] D. Chang et al., Phys. Rev. B 57, 7955 (1998).
[6] L. P. Gor’kov, Zh. Eksp. Teor. Fiz. 37, 833 (1959) [Sov. Phys.-JETP 10, 593 (1960)].
[7] E. Helfand and N. R. Werthamer, Phys. Rev. Lett. 13, 686 (1964).
[8] R. A. Klemm and K. Scharnberg, Phys. Rev. B 24, 6361 (1981).
[9] S. Takahashi and M. Tachiki, Phys. Rev. B 33, 4620 (1986).
[10] V. M. Galitski and S. D. Sarma, Phys. Rev. B 67, 144501 (2003).
[11] A. J. Berlinsky et al., Phys. Rev. Lett. 75, 2200 (1995).
[12] R. Joynt, Phys. Rev. B 41, 4271 (1990).
[13] M. Planck, Verh. Dt. Phys. Ges. 2, 237 (1900).
[14] W. Heisenberg, Z. Phys. 33, 879 (1925).
[15] E. Schrödinger, Ann. Phys. 79, 489 (1926).
[16] T. Koyama et al., Physica (Amsterdam) 194C, 20 (1992).
[17] J. R. Clem, Supercond. Sci. Technol. 11, 909 (1998).
[18] W. E. Lawrence and S. Doniach, in Proc. 12th Int. Conf. on Low Temperature Physics, edited by E. Kanda (Academy, Kyoto, 1971), p. 361.
[19] L. Wang et al., Supercond. Sci. Technol. 14, 252 (2001).
[20] L. Wang et al., Supercond. Sci. Technol. 14, 754 (2001).
[21] L. Wang et al., Physica (Amsterdam) 383C, 247 (2002).
[22] L. Wang, Ph.D. thesis, National University of Singapore, 2002.
[23] V. L. Ginzburg, Zh. Eksp. Teor. Fiz. 31, 541 (1956) [Sov. Phys.-JETP 4, 594 (1957)].
[24] M. Tinkham, Introduction to Superconductivity (McGraw-Hill, New York, 1996).
[25] J. Nagamatsu et al., Nature (London) 410, 63 (2001).
[26] D. K. Finnemore et al., Phys. Rev. Lett. 86, 2420 (2001).
[27] J. A. Woollam et al., Phys. Rev. Lett. 32, 712 (1974).
[28] L. D. Landau and E. M. Lifshitz, Quantum mechanics (non-relativistic theory), translated by J. B. Sykes and J. S. Bell (Pergamon Press, Oxford, 1977).
[29] S. T. Ruggiero et al., Phys. Rev. Lett. 45, 1299 (1980).
[30] S. K. Sundaram and R. Joynt, Phys. Rev. Lett. 66, 512 (1991).
[31] A. S. Alexandrov et al., Phys. Rev. Lett. 76, 983 (1996).
[32] A. A. Abrikosov, Phys. Rev. B 56, 5112 (1997).
[33] S. V. Shulga et al., Phys. Rev. Lett. 80, 1730 (1998).
[34] B. Brandow, Phys. Rep. 296, 1 (1998), and references therein.
[35] L. P. Gor’kov, Zh. Eksp. Teor. Fiz. 31, 1299 (1956).
[36] A. S. Alexandrov et al., Phys. Rev. B 76, 983 (1996).
[37] U. Welp et al., Phys. Rev. B 67, 012505 (2003).
[38] T. Domasi et al., Phys. Rev. B 67, 134507 (2003), and references therein.
[39] A. I. Sokolov, Physica (Amsterdam) 174C, 268 (1991).
[40] L. Wang et al., cond-mat/0201307 and cond-mat/0201321.
[41] D. Saint-James and P. G. Gennes, Phys. Lett. 7, 306
[40] M. Tegmark and J. A. Wheeler, Sci. Am. 284, 68 (2001).
[41] F. Laloë, Am. J. Phys. 69, 655 (2001).
[42] A. J. Leggett, J. Phys.: Condens. Matter 14, R415 (2002).
[43] A. Zeilinger, Nature (London) 408, 639 (2000).