Precision Ginzburg-Landau Solution of Ideal Vortex Lattices for Any Induction and Symmetry

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A method is presented that solves the Ginzburg-Landau equations for the ideal Abrikosov vortex lattice in type-II superconductors with high precision for arbitrary induction, Ginzburg-Landau parameter, and vortex lattice symmetry. This iteration procedure excels previous one-dimensional circular cell methods and approximate variational methods, and is easily adapted to anisotropic and unconventional superconductors. Selected results are given for the order parameter, the form factors of the periodic magnetic field measurable by neutron scattering, reversible magnetization curves, and the shear modulus of the vortex lattice, which could not be obtained by previous methods. [S0031-9007(97)02718-X]

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After Abrikosov's [1] famous solution of the Ginzburg-Landau (GL) equations from which he predicted the existence of a lattice of quantized magnetic vortices in type-II superconductors, much effort has been devoted to extend Abrikosov's approximate analytical solutions, valid at high or low magnetic fields, to the entire field range. From his periodic solution at $B_a \approx \bar{B} \approx B_{c2}$ and the isolated vortex solution at $B_a \to B_{c1}$, $\bar{B} \to 0$, Abrikosov qualitatively obtained the magnetization curve $\bar{B}(B_a)$ in the entire field range and successfully explained the experiments. Here B_a denotes the external field, $\bar{B} = \langle B(x,y)\rangle = \Phi_0/S$ the spatially averaged magnetic field (B_a and $\bar{B}$ are along z) with $\Phi_0 = h/2e$ (or $\Phi_0 = hc/2e$) the quantum of flux and S the area of the lattice cell; $B_{c2} = \Phi_0/(2\pi\xi^2)$ and $B_{c1} \approx (\ln\kappa + 0.5)\Phi_0/(4\pi\lambda^2)$ are the upper and lower critical fields introduced by Abrikosov, ξ is the coherence length, and λ the magnetic penetration depth of the GL theory defining the GL parameter $\kappa = \lambda/\xi$. Type-II superconductors exhibit $\kappa \geq 1/\sqrt{2}$.

A first analytical extension of the B_{c2} solution was elaborated by Eilenberger [2], but this complex series expansion applies only in a narrow field range below B_{c2}. The numerical extension of the B_{c1} (isolated vortex) solution by Ihle [3], approximating the hexagonal Wigner-Seitz cell of the vortex lattice by a circle, applies to the entire field range and even yields the correct B_{c2} value. This circular cell method computes rather accurate magnetization curves, but, in principle, cannot give the energy difference between various lattice symmetries, the shear modulus of the triangular lattice, and the form factors (Fourier coefficients) of the periodic magnetic field $B(x,y)$, which near B_{c2} should have alternating signs. This restriction applies also to Clem's [4] elegant method, which at $\bar{B} \ll B_{c2}$ approximates the GL order parameter $|\psi(x,y)|^2$ by the trial function $r^2/(r^2 + \xi_v^2)$ ($r^2 = x^2 + y^2$) that allows an analytic solution of the second GL equation for $B(x,y)$; the vortex core radius ξ_v is then determined by minimizing the GL free energy. This one-dimensional (1D) variational method was generalized to larger reduced inductions $b = \bar{B}/B_{c2}$ by Hao *et al.* [5]. The Clem-Hao $B(x,y)$ at $b \ll 1$ and $\kappa \gg 1$ is an excellent approximation to the exact GL result obtained below.

A variational method, which, in principle, allows one to compute the periodic GL solution to any desired accuracy, was developed in Ref. [6] by expressing the GL free energy F in terms of the real and periodic functions $B(x,y)$ and $\omega(x,y) = |\psi(x,y)|^2$ [the complex GL function $\psi(x,y)$ is not periodic and not gauge invariant] and minimizing F with respect to a finite number of Fourier coefficients. At that time, computer efficiency allowed only for a small number of variational parameters, one for ω and up to five for B, restricting such computations to $b = \bar{B}/B_{c2} \geq 0.1$. The numerical effort of such a minimization of F increases with a high power of the number of variational parameters, and it is not very precise due to rounding errors.

This Letter presents an iteration method which overcomes these restrictions and allows one to compute over 1000 Fourier coefficients of $B(x,y)$ and $\omega(x,y)$ with high precision even on a personal computer. The method applies down to very low inductions $10^{-3} \leq b < 1$, to arbitrary symmetry of the vortex lattice, and to all relevant GL parameters $1/\sqrt{2} \leq \kappa < \infty$. This genuine two-dimensional (2D) method allows one to compute, for the first time, the shear modulus c_{66} and the form factors of the triangular (and any other) vortex lattice in isotropic and anisotropic GL superconductors for any value of b and κ. Here we describe this method for conventional isotropic GL superconductors and present some selected results.

We start from the average GL free energy density

$$\frac{F}{V} = f = \left\langle -|\psi|^2 + \frac{|\psi|^4}{2} + \left| \left(\frac{\nabla}{i\kappa} - \mathbf{A} \right) \psi \right|^2 + B^2 \right\rangle \tag{1}$$

in the usual reduced units B_c^2/μ_0 (or $B_c^2/4\pi$) for f, $\sqrt{2}\,B_c$ for B, and λ for lengths, with $B_c = \Phi_0/(\sqrt{8}\,\pi\,\xi\,\lambda)$ the

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thermodynamic critical field. $\mathbf{A}$ is the vector potential and $\mathbf{B} = \hat{\mathbf{z}}B = \nabla \times \mathbf{A}$ the local field. In these units, one has $\xi = 1/\kappa$, $B_{c2} = \kappa$, and $\Phi_0 = 2\pi/\kappa$. Writing the GL function as $\psi(x,y) = \omega(x,y)^{1/2}\exp[i\varphi(x,y)]$, with $\omega = |\psi|^2 \le 1$ and introducing the supervelocity $\mathbf{Q}(x,y) = \mathbf{A}(x,y) - \nabla\varphi(x,y)/\kappa$, we may write f in terms of the gauge invariant real functions $\omega(x,y)$ and $\mathbf{Q}(x,y)$,

$$f = \left\langle -\omega + \frac{\omega^2}{2} + \frac{(\nabla\omega)^2}{4\kappa^2\omega} + \omega\mathbf{Q}^2 + (\nabla\times\mathbf{Q})^2 \right\rangle. \tag{2}$$

Without restriction of generality, using only the inversion symmetry of the lattice and assuming one Φ_0 per vortex, we may express ω, B, and $\mathbf{Q}$ as the Fourier series,

$$\omega(\mathbf{r}) = \sum_{\mathbf{K}} a_{\mathbf{K}}(1 - \cos\mathbf{K}\cdot\mathbf{r}), \tag{3}$$

$$B(\mathbf{r}) = \bar{B} + \sum_{\mathbf{K}} b_{\mathbf{K}}\cos\mathbf{K}\cdot\mathbf{r}, \tag{4}$$

$$\mathbf{Q}(\mathbf{r}) = \mathbf{Q}_A(\mathbf{r}) + \sum_{\mathbf{K}} b_{\mathbf{K}}\frac{\hat{\mathbf{z}}\times\mathbf{K}}{K^2}\sin\mathbf{K}\cdot\mathbf{r}, \tag{5}$$

with $\mathbf{r} = (x,y)$; the sums are over all $\mathbf{K}_{mn} \neq 0$. For vortex positions $\mathbf{R} = \mathbf{R}_{mn} = (mx_1 + nx_2, ny_2)$ $(m,n$ integer), the reciprocal lattice vectors are $\mathbf{K} = \mathbf{K}_{mn} = (2\pi/S)(my_2, nx_1 + mx_2)$ with $S = x_1y_2 = \Phi_0/\bar{B}$ the unit cell area. For the triangular lattice, one has $x_2 = x_1/2$, $y_2 = x_1\sqrt{3}/2$, and for the square lattice $x_2 = 0$, $y_2 = x_1$. $\mathbf{Q}_A(x,y)$ is the supervelocity of the Abrikosov B_{c2} solution, which satisfies

$$\nabla\times\mathbf{Q}_A = \left[\bar{B} - \Phi_0\sum_{\mathbf{R}}\delta_2(\mathbf{r}-\mathbf{R})\right]\hat{\mathbf{z}}, \tag{6}$$

where $\delta_2(\mathbf{r}) = \delta(x)\delta(y)$ is the 2D delta function. Formula (6) shows that $\mathbf{Q}_A$ is the velocity field of a lattice of ideal vortex lines but with zero average rotation. Near each vortex center, one has $\mathbf{Q}_A(\mathbf{r}) \approx \hat{\mathbf{z}}\times\mathbf{r}'/(2\kappa r'^2)$ and $\omega(\mathbf{r}) \propto r'^2$ with $\mathbf{r}' = \mathbf{r} - \mathbf{R}$. $\mathbf{Q}_A(\mathbf{r})$ may be expressed as a slowly converging Fourier series by integrating (6) using $\mathrm{div}\mathbf{Q} = \mathrm{div}\mathbf{Q}_A = 0$ [6]. It is, however, more convenient to take $\mathbf{Q}_A$ from the exact relation

$$\mathbf{Q}_A(\mathbf{r}) = \frac{\nabla\omega_A\times\hat{\mathbf{z}}}{2\kappa\omega_A}, \tag{7}$$

where $\omega_A(x,y)$ is the Abrikosov B_{c2} solution given by the rapidly converging series (3) with the coefficients [7,8]

$$a^A_{\mathbf{K}} = -(-1)^{m+mn+n}\exp[-K^2_{mn}S/(8\pi)], \tag{8}$$

in general, and $a^A_{\mathbf{K}} = -(-1)^{\nu}\exp(-\pi\nu\sqrt{3})$ $(\nu = m^2 + mn + n^2)$ for the triangular lattice. The ω_A [Eqs. (3) and (8)] is normalized to $\langle\omega_A(x,y)\rangle = 1$; this yields the strange relation $\sum'_{\mathbf{K}} a^A_{\mathbf{K}} = 1$ for any lattice symmetry. Another strange property of the Abrikosov solution [Eqs. (3) and (8)] is that $(\nabla\omega_A/\omega_A)^2 - \nabla^2\omega_A/\omega_A = 4\pi/S = \mathrm{const}$, although both terms diverge at the vortex positions; this relation follows from (6) and (7) using $\bar{B} = \Phi_0/S = 2\pi/(\kappa S)$. The useful formula (7) may be proven via the complex B_{c2} solution $\psi_A(x,y)$; it means that near B_{c2} the third and fourth terms in f [Eq. (2)] are equal.

Following previous ideas [6], one might compute approximate solutions ω and B by using a finite number of Fourier coefficients $a_{\mathbf{K}}$ and $b_{\mathbf{K}}$ and minimizing $f(B,\kappa,a_{\mathbf{K}},b_{\mathbf{K}})$ with respect to these coefficients. However, a much faster and more accurate solution method is to iterate the two GL equations $\delta f/\delta\omega = 0$ and $\delta f/\delta\mathbf{Q} = 0$ written in an appropriate form. Namely, the iteration is stable and converges rapidly if one isolates a term $(-\nabla^2 + \mathrm{const})(\omega, B, \mathbf{Q})$ on the left-hand side and puts the remaining terms to the right-hand side as a kind of "inhomogeneity" of such London-like equations, e.g.,

$$(-\nabla^2 + 2\kappa^2)\omega = 2\kappa^2(2\omega - \omega^2 - \omega Q^2 - g), \tag{9}$$

$$(-\nabla^2 + \bar{\omega})\mathbf{Q}_b = -\omega\mathbf{Q}_A - (\omega - \bar{\omega})\mathbf{Q}_b, \tag{10}$$

with the abbreviations $g = (\nabla\omega)^2/(4\kappa^2\omega)$, $\mathbf{Q}_b = \mathbf{Q} - \mathbf{Q}_A$, $\nabla\times\mathbf{Q}_b = B - \bar{B}$, and $\bar{\omega} = \langle\omega\rangle = \sum_{\mathbf{K}} a_{\mathbf{K}}$. In (9) and (10) I introduced the "penetration depths" $(2\kappa^2)^{-1/2} = \xi/\sqrt{2}$ and $\bar{\omega}^{-1/2} = \lambda/\bar{\omega}^{1/2}$ (in real units) which stabilize the convergence. Acting on the Fourier series ω [Eq. (3)] and $\mathbf{Q}_b$ [Eq. (5)], the Laplacian ∇^2 yields a factor $-K^2$; this makes the inversion of (9) and (10) trivial. Using the orthogonality of the functions $\cos\mathbf{K}\cdot\mathbf{r}$, one obtains from Eqs. (3) and (4) $a_{\mathbf{K}} = -2\langle\omega(\mathbf{r})\cos\mathbf{K}\cdot\mathbf{r}\rangle$ and $b_{\mathbf{K}} = 2\langle B(\mathbf{r})\cos\mathbf{K}\cdot\mathbf{r}\rangle$. The convergence of the iteration is considerably improved by adding a third equation which minimizes f [Eq. (2)] with respect to the amplitude of ω; this step gives the largest decrease of f. The resulting three iteration equations for the parameters $a_{\mathbf{K}}$ and $b_{\mathbf{K}}$ read

$$a_{\mathbf{K}} := \frac{4\kappa^2\langle(\omega^2 - 2\omega + \omega Q^2 + g)\cos\mathbf{K}\cdot\mathbf{r}\rangle}{K^2 + 2\kappa^2}, \tag{11}$$

$$a_{\mathbf{K}} := a_{\mathbf{K}}\cdot\langle\omega - \omega Q^2 - g\rangle/\langle\omega^2\rangle, \tag{12}$$

$$b_{\mathbf{K}} := \frac{-2\langle[\omega B + \bar{\omega}(B-\bar{B}) + p]\cos\mathbf{K}\cdot\mathbf{r}\rangle}{K^2 + \bar{\omega}}, \tag{13}$$

with $p = (\nabla\omega\times\mathbf{Q})\hat{\mathbf{z}} = Q_x\partial\omega/\partial y - Q_y\partial\omega/\partial x$ and $g = (\nabla\omega)^2/(4\kappa^2\omega) = (\nabla|\psi|/\kappa)^2$ as above.

Very stable and fast convergence for any b and κ value is obtained by starting with $a_{\mathbf{K}} = a^A_{\mathbf{K}}$ (8) and $b_{\mathbf{K}} = 0$, then iterating Eqs. (11), (12), (11), (12), etc., a few times to relax ω, and then allowing also B to relax by iterating (11), (12), (13),..., (11), (12), (13). After typically 25 such triple steps, the solution stays constant to all 15 digits and the GL equations are thus satisfied.

Figure 1 shows the resulting profiles of ω and B for $\kappa = 1.5$ since the spatial variation of B is more visible at low κ, see also Fig. 3 below. The shape of the order

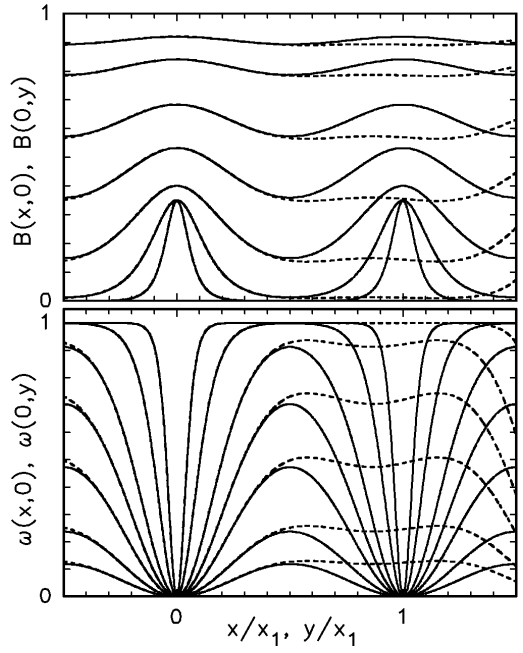

FIG. 1. Profiles of order parameter $\omega(x,y)$ and magnetic field $B(x,y)/B_{c2}$ along the x axis (solid lines) and y axis (dashed lines) for a triangular vortex lattice at reduced inductions $b = \bar{B}/B_{c2} = 0.9, 0.8, 0.6, 0.4, 0.2, 0.05, 0.01$ for $\kappa = 1.5$.

parameter ω is qualitatively the same for all $1/\sqrt{2} \le \kappa < \infty$, with a narrower vortex core at smaller κ.

For each set of parameters b, κ, x_2/x_1, and y_2/x_1, the computation takes a few seconds on a Pentium PC. Since all terms in (11)–(13) are smooth periodic functions of $\mathbf{r}$, high accuracy is achieved on an equidistant 2D grid, e.g., $x_i = (i - 1/2)x_1/N_x \quad (i = 1,\ldots,N_x)$ and $y_j = (j - 1/2)y_2/(2N_y) \quad (j = 1,\ldots,N_y, 2N_y \approx N_x y_2/x_1)$. These $N = N_x N_y = 100$–1000 grid points fill the rectangular basic area $0 \le x \le x_1$, $0 \le y \le y_2/2$, valid for any parallelogram unit cell. Averaging $\langle\ldots\rangle$ then just means summing N terms with constant weight $1/N$. I consider all $\mathbf{K}_{mn}$ vectors in a half circle $|\mathbf{K}_{mn}| \le K_{\max}$ with $K_{\max}^2 \approx 20N/S$ chosen such that the number M of the $\mathbf{K}_{mn}$ is slightly less than the number N of grid points. The $M \times N$ matrices $\cos \mathbf{K}\cdot\mathbf{r}$ and $\sin \mathbf{K}\cdot\mathbf{r}$ are tabulated.

The high precision of this method may be checked with the identity $B(x,y)/B_{c2} = 1 - \omega(x,y)$, which is valid at $\kappa = 1/\sqrt{2}$ for all b; this is confirmed with error $<10^{-9}$.

To obtain the equilibrium applied field B_a or reversible magnetization $M = \bar{B} - B_a$, one may use the relation $B_a = \partial f/\partial \bar{B}$. A much more convenient way, which circumvents taking the numerical derivative of the free energy density f [Eq. (2)], is to use the virial theorem discovered recently by Doria, Gubernatis, and Rainer [9], who found that (still in units of $\sqrt{2}\,B_c$)

$$B_a = \langle \omega - \omega^2 + 2B^2 \rangle / \langle 2B \rangle . \qquad (14)$$

This useful discovery shows that GL equations and the Abrikosov solution are still active. Reversible magnetization curves obtained in this way are depicted in Fig. 2, confirming the qualitative curves given, e.g., in the reviews [10,11]. For comparison with muon-spin rotation experiments, the field $B_{\max}$ at the vortex centers, the minimum field $B_{\min}$, and the external field B_a are plotted in Fig. 3 versus $b = \bar{B}/B_{c2}$ for various κ values. Note that the field in the vortex center always exceeds the external field;

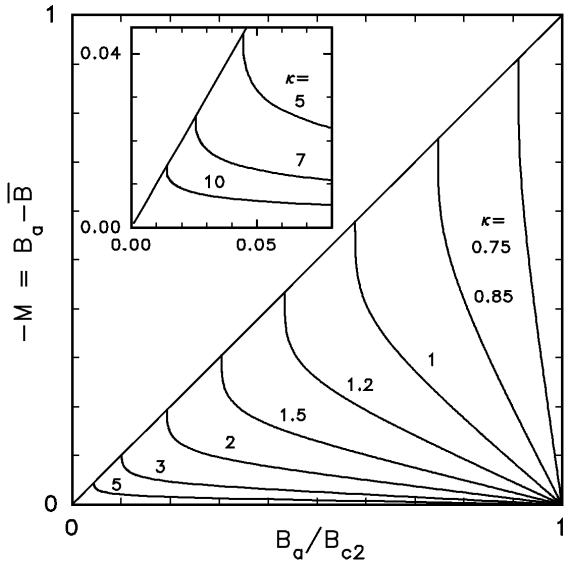

FIG. 2. Reversible magnetization curves of ideal vortex lattices in units B_{c2}. The curves for the triangular and square lattices coincide within line thickness and thus cannot be distinguished in this plot.

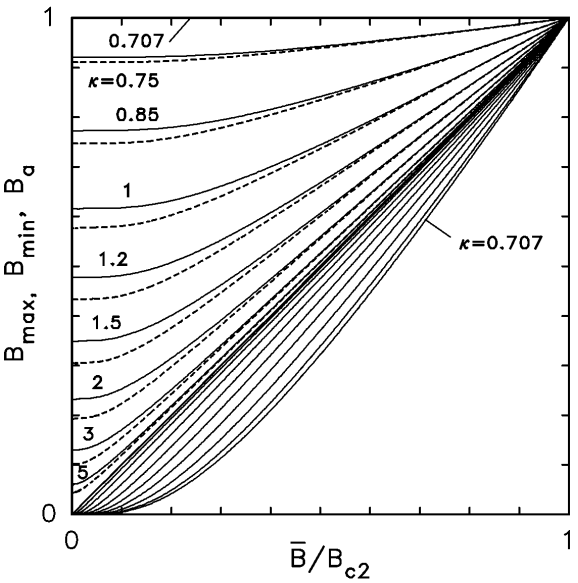

FIG. 3. The maximum magnetic field $B_{\max}$ (upper solid lines) occurring at the vortex centers and the minimum field $B_{\min}$ (lower solid lines) of the triangular vortex lattice compared with the applied field B_a (dashed lines) and average induction $\bar{B}$ (diagonal line) in units B_{c2}, plotted versus $b = \bar{B}/B_{c2}$ for $\kappa = \sqrt{0.5}$, 0.75, 0.85, 1, 1.2, 1.5, 2, 3, and 5.

TABLE I. The first five Fourier coefficients $b_{\mathbf{K}} = b_{mn}$ (4) of the triangular vortex lattice in the limit $\kappa \gg 1$ divided by the London limit $b_{\mathbf{K}} = \bar{B}/(1 + K^2\lambda^2)$.

$\bar{B}/B_{c2}$	b_{10}	b_{11}	b_{20}	b_{21}	b_{30}
0.990	0.0051	0.0004	−0.00009	0.00000	0.00000
0.950	0.0256	0.0021	−0.00038	0.00000	0.00000
0.900	0.0514	0.0045	−0.00061	0.00002	0.00000
0.800	0.1036	0.0099	−0.00052	0.00009	0.00000
0.700	0.1570	0.0168	0.00058	0.00025	0.00002
0.600	0.2121	0.0259	0.00319	0.00059	0.00008
0.500	0.2699	0.0382	0.00826	0.00133	0.00026
0.400	0.3322	0.0563	0.01767	0.00297	0.00078
0.300	0.4026	0.0853	0.03572	0.00703	0.00239
0.200	0.4901	0.1394	0.07475	0.01914	0.00828
0.100	0.6241	0.2710	0.18558	0.07250	0.04152
0.050	0.7415	0.4391	0.34751	0.18871	0.13119
0.020	0.8579	0.6564	0.58224	0.42135	0.34628
0.010	0.9139	0.7805	0.72679	0.59793	0.53028
0.005	0.9483	0.8630	0.82677	0.73408	0.68164
0.002	0.9718	0.9238	0.90252	0.84514	0.81050
0.001	0.9796	0.9471	0.93201	0.89037	0.86524

for $b \ll \kappa^{-2} \ll 1$, one has $B_{\max} = 2B_a = 2B_{c1}$, but near B_{c2} the difference, $B_{\max} - B_a \propto (1 - b)^2$, is small while the magnetization, $\bar{B} - B_a = M \propto 1 - b$, is larger.

I list now some new results which could not be obtained by previous methods. Note that so far our knowledge of the properties of the vortex lattice was almost entirely based on the low field and high field approximations, whose accuracy was not known in principle. One striking example is discussed in Ref. [12], namely, the pronounced cusplike $\bar{B}$ dependence of the form factors $b_{\mathbf{K}}$ at very low inductions $\bar{B} \ll B_{c2}$, where the London theory predicts $\bar{B}$ independence.

For comparison with neutron scattering experiments, the first five magnetic form factors $b_{\mathbf{K}}$ [Eq. (4)] are given in Table I. Note the negative sign of b_{20} at $b \geq 0.75$, in agreement with Abrikosov [1], and the correct attainment of the London limit $b_{\mathbf{K}} = \bar{B}/(1 + K^2\lambda^2)$ for $b \ll 1$. At $b = 0.01$ and $\kappa \gg 1$, the first five $b_{\mathbf{K}}$ deviate by only (3, 3, 2, 0, −2)% from the Clem-Hao approximation [4,5] given explicitly in Ref. [12].

When the shape of the unit cell is varied periodically from triangular to rectangular (if $y_2 = \sqrt{3}\,x_1/2$) or from square to rectangular (if $y_2 = x_1$) by increasing x_2 continuously, then the free energy is found to vary almost exactly sinusoidally, e.g., $f(x_2) = f_0 + [1 + \cos(2\pi x_2/x_1)]f_1$ for the triangular lattice. The shear modulus of this vortex lattice is thus $c_{66} = y_2^2\partial^2 f/\partial x_2^2 = 3\pi^2 f_1$ or

$$c_{66} = (3\pi^2/2)[f(x_2 = 0) - f(x_2 = x_1/2)]. \quad (15)$$

This exact shear modulus, shown in Fig. 4, looks qualitatively like the approximate c_{66} estimated from an effective vortex interaction in Ref. [13], but its maximum value $c_{66}^{\max} = 0.0415B_c^2/\mu_0$ (at $b = 0.295$, $\kappa \geq 10$) is about 15% smaller. For $\kappa \geq 10$, one has at $b \ll \kappa^{-2}$: $c_{66} \propto \exp(-\text{const}/\sqrt{b})$, at $\kappa^{-2} \ll b \ll 1$: $c_{66} \approx b/4$, and at $b \geq 0.7$: $c_{66} \approx 0.177(1 - b)^2$ in units B_c^2/μ_0, in agreement with the analytic result [7,13,14].

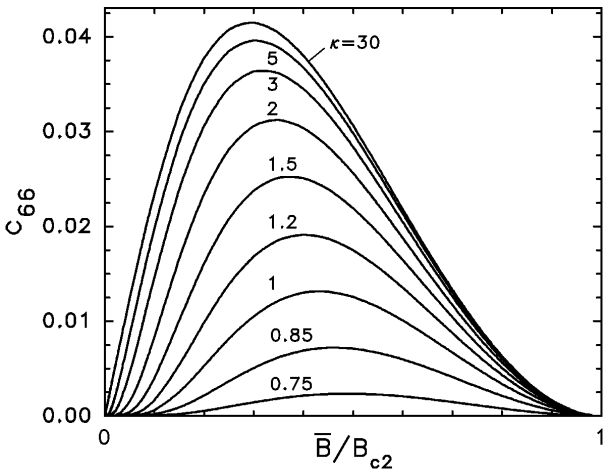

FIG. 4. The shear modulus c_{66} of the triangular vortex lattice in units B_c^2/μ_0, plotted versus b for $\kappa = 0.75$, 0.85, 1, 1.2, 1.5, 2, 3, 5, and 30, equivalent to $\kappa = \infty$.

In conclusion, our novel iteration method to obtain the 2D periodic solutions of the isotropic or anisotropic GL equations supplements the 1D circular cell method [3] and surpasses in precision the 2D variational method [6]. It allows one, for the first time, to calculate in the entire field range $0 < \bar{B} < B_{c2}$ the form factors of magnetic field and order parameter, and the free energy and shear modulus of vortex lattices with given symmetry. Discussion of these results, analytic fits, and the extension to anisotropic superconductors will be given elsewhere.

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