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Vortex-lattice solutions of the microscopic Gorkov equations for a type-II superconductor in a strong quantizing magnetic field

J. C. Ryan and A. K. Rajagopal
Naval Research Laboratory, Washington, D.C. 20375-5000
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We derive solutions of the Gorkov equations for a type-II superconductor using the fact that the vortex lattice is a consequence of translation and gauge covariance. We thus generalize the Abrikosov solutions of the vortex lattice to include Cooper pairing in higher-order Landau indices relevant to low temperatures and high quantizing second critical fields where the semiclassical assumptions of the Ginzburg-Landau theory break down. Detailed calculations of the pairing amplitudes are presented for triangular and square lattices in a diagonal Landau-state approximation illustrating the effects of temperature and magnetic field on the vortex lattices. These solutions are also of interest because they give a purely microscopic view of the vortex lattice and the correlations responsible for it.

I. INTRODUCTION

The discovery of the vortex lattice solutions within the Ginzburg-Landau (GL) theory of type-II superconductivity by Abrikosov[1] in 1957 has spawned a large variety of investigations.[2,3] Most of these are based on the semiclassical approximation for the effects of a magnetic field within the GL theory. The underpinning of all this is the well-known microscopic theory of Gorkov within a BCS scheme from which the GL theory follows as an approximation near the superconducting phase transition.[4,5]

Recent advances in scanning tunneling microscopy[6] and high-field magnets[7] have opened new windows on the electronic structure of the vortex state, generating hope of eventually accessing the regime of quantized cyclotron orbits.[8,9] This would be of great interest because recent theoretical investigations by several authors[10,11] have pointed toward the possible coexistence of superconductivity and high fields by showing that the superconducting state for a spinless electron persists well above the semiclassical phase boundary. Further analysis by Rieck *et al.*[12] have shown that a nonzero paramagnetic g factor is detrimental to this state although the above phase boundary is still quite unlike that predicted by the semiclassical theory.

Investigations of the vortex lattice within this context, using the Bogoliubov-de Gennes equations, have only recently appeared[13] and employ a two-dimensional model in the extreme high-field limit—only a single Landau level within the shell of attraction. Except for the ground level, this assumption is violated of necessity in three dimensions because of the momentum dispersion along the field direction, and the mean-field theory is known to be suspect in two dimensions. Other authors[14] have also employed the Bogoliubov-de Gennes formalism. However, this formalism is not readily generalizable to include strong-coupling interactions needed to incorporate the alterations in the effective phonon and Coulomb-mediated interelectron interactions that would certainly appear at such high fields.[15] Attempts to self-consistently include the induced magnetic field have also been made,[16] but only a single vortex has thus far been considered.

The purpose of the present work is to construct the vortex lattice solutions of the Gorkov equations in the presence of a quantizing magnetic field within a constant-field BCS model, thereby providing a consistent theory applicable over the whole phase boundary, and as far below it as the constant-field assumption will allow. This not only enables calculation of detailed electronic structure, but also provides insight into the microscopic detail of the correlations responsible for the vortex lattice.

We construct the vortex lattice by exploiting the translation and gauge covariance of the Gorkov equations.[17] It is well known that a translationally invariant superconducting state in a magnetic field is impossible because of the destructive interference of the Aharanov-Bohm phases between electron pairs. However, a superconducting state invariant under a discrete set of translations is possible if translation around any closed path encloses an integral number of flux quanta. This is the condition for constructive interference of the Aharanov-Bohm phases. In this way, the lattice is formed by correlations among electrons whose orbit centers satisfy the above condition, while pairing is suppressed among all others. It follows that, unlike the semiclassical approximation where the magnetodynamics of the internal Cooper pair motion is not discernible, we find that the relative or intrapair correlations consistent with the formation of a lattice are essential in determining the superconducting state. We also find the form of the original Abrikosov solution to be a special case of the solution presented here, in which Cooper pairs occupy only the lowest Landau level.

The importance of these results is threefold. One, it gives an intrinsically microscopic view of how the vortex lattice is formed from the states of the normal system; two, it applies to the basically quantum regimes that may soon be accessible in both the low-T_c and high-T_c superconductors where Landau quantization effects cannot be

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ignored,[18,19] and three, it applies to low temperature where the semiclassical approximations break down. We begin in Sec. II by presenting the translation and gauge properties of the Gorkov equations, and use these properties in Sec. III to identify the electrons whose correlations readily give rise to pairing. In Sec. IV we illustrate the solution within a simple diagonal approximation, and conclude with some remarks on applicability and future directions in Sec. V. In the Appendix we give the transformation properties of the Landau states under rotations and the associated implications for the square and triangular vortex lattices.

II. TRANSLATION COVARIANCE

We begin with a discussion of the covariance of the Gorkov equations.[17] The equations are

$$[i\omega_\nu-\hat{H}_0(\mathbf{A})]G(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)-\Delta(\mathbf{r}_1)F^\dagger(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)=\delta(\mathbf{r}_1-\mathbf{r}_2)\ , \quad (1a)$$

$$[-i\omega_\nu-\hat{H}_0^*(\mathbf{A})]F^\dagger(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)+\Delta^\dagger(\mathbf{r}_1)G(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)=0\ , \quad (1b)$$

$$\nabla\times[\nabla\times\mathbf{A}(\mathbf{r})]=\frac{i}{2m}\lim_{t\to 0^-}\lim_{\mathbf{r}'\to\mathbf{r}}\left[\left[-i\hbar\nabla_{\mathbf{r}}+\frac{e\,\mathbf{A}(\mathbf{r})}{c}\right]+\left[i\hbar\nabla_{\mathbf{r}'}+\frac{e\,\mathbf{A}(\mathbf{r}')}{c}\right]\right]\times G(\mathbf{r},\mathbf{r}';t)\ . \quad (1c)$$

Here

$$\hat{H}_0(\mathbf{A})=[-i\hbar\nabla_{\mathbf{r}}+e\,\mathbf{A}(\mathbf{r})/c]^2/2m\ , \quad (2a)$$

$$\Delta(\mathbf{r})=-\frac{\overline{V}}{\beta}\sum_\nu F(\mathbf{r},\mathbf{r};i\omega_\nu)\ , \quad (2b)$$

ω_ν being the usual Matsubara frequency and $\overline{V}$ is the attractive interaction that promotes Cooper pair formation in the BCS scheme within an energy shell around the Fermi surface. In the extreme type-II systems of our interest, the spatial variation of the magnetic field, $\mathbf{H}(\mathbf{r})=\nabla\times\mathbf{A}(\mathbf{r})$ (penetration depth λ), is slow compared to those of the superconducting correlations (coherence length ξ) so that $\mathbf{H}(\mathbf{r})$, to a good approximation, may be taken to be constant, and $\mathbf{A}(\mathbf{r})$ may be chosen to be linear in $\mathbf{r}$. In the above equations spin has been neglected but may easily be incorporated by including the Zeeman term in the Hamiltonian, whereby G, F, and Δ carry spin indices as well.

The most important observation is that if G, $F^\dagger$, Δ, $\Delta^\dagger$ are solutions of the above equations, and we translate $\mathbf{r}_1$ and $\mathbf{r}_2$ by a constant vector, then $\tilde{G}$, $\tilde{F}^\dagger$, $\tilde{\Delta}$, $\tilde{\Delta}^\dagger$ defined by the following set:

$$\tilde{G}(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)=\exp[ie(\mathbf{r}_1-\mathbf{r}_2)\cdot\mathbf{A}(\mathbf{a})/\hbar c]\times G(\mathbf{r}_1+\mathbf{a},\mathbf{r}_2+\mathbf{a};i\omega_\nu)\ , \quad (3a)$$

$$\tilde{F}^\dagger(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)=\exp[-ie(\mathbf{r}_1+\mathbf{r}_2)\cdot\mathbf{A}(\mathbf{a})/\hbar c]\times F^\dagger(\mathbf{r}_1+\mathbf{a},\mathbf{r}_2+\mathbf{a};i\omega_\nu)\ , \quad (3b)$$

$$\tilde{\Delta}^\dagger(\mathbf{r})=\exp[-i2e\mathbf{r}\cdot\mathbf{A}(\mathbf{a})/\hbar c]\Delta^\dagger(\mathbf{r}+\mathbf{a})\ , \quad (3c)$$

are also solutions of the same Gorkov equations. This is the fundamental covariance of the Gorkov equations under the combined translation and gauge transformation (magnetic translation group), showing the translation-induced Aharanov-Bohm phases. Notice that the phase of the pair correlation function, $F^\dagger$, depends upon the center of mass of the pair, $(\mathbf{r}_1+\mathbf{r}_2)/2$, with charge $2e$. These are then the position and charge of the Cooper pair.

We now choose $\mathbf{A}(\mathbf{r})=\mathbf{H}\times\mathbf{r}/2, \mathbf{H}=(0,0,H)$ and employ the orbit center representation for the solutions of $\mathbf{H}_0(\mathbf{A})$ as in Ref. 19, where for simplicity, we focus on the two dimensions perpendicular to the field, leaving the possibility of including other isotropic or layered structures in the third dimension:[19,20]

$$\hat{H}_0(\mathbf{A})\psi_{NX}(\mathbf{r})=\varepsilon_N\psi_{NX}(\mathbf{r})\ , \quad (4a)$$

$$\psi_{NX}(\mathbf{r})=\exp(ixy/2l^2)\exp(-iXy/l^2)\phi_N(x-X)\ , \quad (4b)$$

where X is the orbit center, N is the Landau quantum number, $\{\phi_N\}$ are the orthonormal harmonic oscillator eigenfunctions, $\varepsilon_N=\hbar\omega_c(N+1/2)$ are the Landau-level energies, and the cyclotron frequency and Larmor radius are respectively defined as

$$\omega_c=eH/mc\ ,\quad l^2=c\hbar/eH\ .$$

III. LATTICE SOLUTIONS

We now use the above set of states as our basis to expand the anomalous Green's function F, suitably adopted to a lattice reflecting the translation properties discussed in Sec. II. For a stable configuration, the only nonzero pair correlations will be those between electron states whose center of mass satisfies the proper constructive Aharonov-Bohm interference condition, $X_1=ma_x/M+X$ and $X_2=ma_x/M-X$, where m is an integer. This defines a subset of the translation group that defines a lattice with periods a_x and $a_y=M\pi l^2/a_x$ where M is an integer that determines the number of flux quanta per unit cell.

Similarly, a single electron propagating in the presence of such periodic pairing can only be scattered into a state differing from the original by a reciprocal lattice vector. Since the orbit center X is equivalent to the momentum in the y direction we must have $\Delta X/l^2=2\pi m/a_y$, where m is an integer. This is used in expressing G in terms of the above set of states by restricting the orbit centers to $X_1=X+\pi l^2m/a_y$ and $X_2=X-\pi l^2m/a_y$. These constraints satisfy the translation properties [Eqs. (3a), (3b)] and the following expansions for the Green's functions are obtained (where we have used $a_x/M=\pi l^2/a_y$):

$$G(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)=\sum_{N_1N_2}\sum_m\int\frac{dX}{2\pi l^2}\psi_{N_1,X+a_xm/M}(\mathbf{r}_1)\psi^*_{N_2,X-a_xm/M}(\mathbf{r}_2)G_{N_1N_2}(X,m;i\omega_\nu)\ , \tag{5a}$$

$$F^\dagger(\mathbf{r}_1,\mathbf{r}_2;i\omega_\nu)=\sum_{N_1N_2}\sum_m\int\frac{dX}{2\pi l^2}\psi^*_{N_1,ma_x/M+X}(\mathbf{r}_1)\psi^*_{N_2,ma_x/M-X}(\mathbf{r}_2)F^\dagger_{N_1N_2}(m,X;i\omega_\nu)\ . \tag{5b}$$

The lattice periodicity is achieved by requiring

$$F^\dagger_{N_1N_2}(m+M,X;i\omega_\nu)=F^\dagger_{N_1N_2}(m,X;i\omega_\nu) \tag{6a}$$

and

$$G_{N_1N_2}(X+a_x,m;i\omega_\nu)=G_{N_1N_2}(X,m;i\omega_\nu)\ . \tag{6b}$$

The values of M and the ratio of a_x/a_y as well as the relationship between the M different $F^\dagger$ functions determine the geometry of the lattice.

The resulting form of Δ is best illustrated by using the transformation to relative and center-of-mass coordinates, i.e.,

$$\psi_{N_1,ma_x/M+X}(\mathbf{r}_1)\psi_{N_2,ma_x/M-X}(\mathbf{r}_2)=\sum_P^{N_1+N_2}C^P_{N_1N_2}\psi^{\rm cm}_{P,ma_x/M}(\mathbf{r}_{\rm cm})\psi^{\rm rel}_{N_1+N_2-P,2X}(\mathbf{r}_{\rm rel})\ , \tag{7}$$

where

$$C^P_{N_1N_2}=\left[\frac{P!(N_1+N_2-P)!}{N_1!N_2!}\right]^{1/2}\frac{(-1)^{N_2}}{2^{(N_1+N_2)/2}}\times\sum_{j=0}^P(-1)^j\begin{bmatrix}N_1\\P-j\end{bmatrix}\begin{bmatrix}N_2\\j\end{bmatrix}\ , \tag{8}$$

$\mathbf{r}_{\rm cm}=(\mathbf{r}_1+\mathbf{r}_2)/2$, $\mathbf{r}_{\rm rel}=\mathbf{r}_1-\mathbf{r}_2$, and the functions $\psi^{\rm cm}$ and $\psi^{\rm rel}$ have the same form as Eq. (4b) but with the associated magnetic length l replaced by $2^{-1/2}l$ and $2^{1/2}l$, respectively. It can then be seen that the gap function Δ quite generally takes the form

$$\Delta^\dagger(\mathbf{r})=\sum_{P,m}\psi^{\rm cm*}_{P,ma_x/M}(\mathbf{r})A^P(m)\ , \tag{9}$$

where the coefficients $A^P(m)$ are defined by

$$A^P(m)=-2^{-1/2}\sum_{N_1N_2}C^P_{N_2N_1}\int\frac{dX}{2\pi l^2}\phi^{\rm cm}_{N_1+N_2-P}(X)\frac{\overline{V}}{\beta}\sum_\nu F^\dagger_{N_1N_2}(m,X;i\omega_\nu) \tag{10}$$

and

$$A^P(m+M)=A^P(m)$$

follows from Eq. (6a). [Here we have used $\phi^{\rm rel}(2X)=2^{-1/2}\phi^{\rm cm}(X)$]. The problem of determining the structure of the order parameter is therefore reduced to a self-consistent calculation of the coefficients A^P. We would like to emphasize here that P is the Landau index of the Cooper pair and A^P is the probability amplitude of finding a Cooper pair in the $P^{\rm th}$ Landau level. P has nothing to do with angular momentum.[13] The $A^P(m)$ coefficients can be compared to the expansion coefficients C_m in the Abrikosov solution (Refs. 1 and 21). The Abrikosov expansion is a variational solution for which the Cooper pairs are all in the lowest Landau level, and therefore $P=0$ is implicit in all the C_m coefficients.

The determination of $\{A^P\}$ proceeds by solving the Gorkov equations using the above constructions [Eq. (5)] with F and Δ self-consistently connected via $\{A^P\}$ through Eqs. (9) and (10). The Gorkov equations acquire the following form:

$$G_{N_1N_2}(X,m;i\omega_\nu)=G^0_{N_1}(i\omega_\nu)\delta_{N_1N_2}\delta_{m,0}+G^0_{N_1}(i\omega_\nu)\sum_{N_3}\sum_{m'}\Delta_{N_1N_3}(m+m',X-m'a_x/M)\times F^\dagger_{N_3N_2}(m',(m'+m)a_x/M-X;i\omega_\nu)\ ; \tag{11a}$$

$$F^\dagger_{N_1N_2}(m,X;i\omega_\nu)=-G^0_{N_1}(-i\omega_\nu)\sum_{N_3}\sum_{m'}\Delta^\dagger_{N_1N_3}(m'+m,X-a_xm'/M)G_{N_3N_2}((m'+m)a_x/M-X,m';i\omega_\nu)\ , \tag{11b}$$

where the integral of $\Delta(r)$, using Eqs. (7) and (9), is

$$\Delta_{N_1N_2}(m,X)=2^{-1/2}\sum_P C^P_{N_2N_1}\phi^{\rm cm}_{N_1+N_2-P}(X)A^P(m)\ , \tag{11c}$$

and it should always be remembered that the Landau-index sums are restricted to values lying within the energy shell. We note that the free-particle Green's function is correctly obtained from the first term in Eq. (11a). For $M=1$ and $M=2$ (corresponding to the square and triangular lattices), this set of equations can be diagonalized in m with the following transformations:

$$G_{N_1N_2}(\mathbf{R};i\omega_\nu)=\sum_m e^{-2\pi imY/a_y}G_{N_1N_2}(X+a_xm/M,m;i\omega_\nu)\ , \tag{12a}$$

$$F^\dagger_{N_1N_2}(\mathbf{R};i\omega_\nu)=e^{iYX/l^2}\sum_m e^{-2\pi imY/a_y}F^\dagger_{N_1N_2}(m,ma_x/M-X;i\omega_\nu)\ , \tag{12b}$$

$$\Delta_{N_1N_2}(\mathbf{R})=e^{-iYX/l^2}\sum_m e^{2\pi imY/a_y}\Delta_{N_1N_2}(m,X-ma_x/M) \tag{12c}$$

with a definition for $\Delta^\dagger$ similar to that of $F^\dagger$, which yields, from Eq. (11c),

$$\Delta^\dagger_{N_1N_2}(\mathbf{R})=\sum_P C^P_{N_1N_2}\sum_m A^P(m)\psi^{\mathrm{cm}*}_{N_1+N_2-P,ma_x/M}(\mathbf{R})\ . \tag{13}$$

We see that $G(R)$ is periodic while F is quasiperiodic[21] in X and Y with respective periods a_x and a_y. We note that $\mathbf{R}$ defines the magnetic Brillouin zone.

For present purposes, the cases of $M=1$ with $a_x=a_y$ and $M=2$ with $a_x=3^{1/2}a_y$ (or $a_x=a_y/3^{1/2}$) are all that are needed to include the square[1] and triangular[22] lattices, respectively. Insisting upon equivalence of lattice and basis points in the triangular lattice[21] defines the connection between the two distinct $A^P(m)$ coefficients: $A^P(1)=-iA^P(0)$. We will therefore find it convenient to write $A^P(m)=\exp(-i\theta_m)A^P$ with $\theta_m=\pi m^2/2$ and express the order parameter in the form

$$\Delta(\mathbf{r})=\sum_P A^P\sum_m \exp(-i\theta_m)\psi^{\mathrm{cm}}_{P,ma_x/M}(\mathbf{r})$$
$$\equiv\sum_P A^P\Delta^P(\mathbf{r})\ .$$

The integro-matrix equations are thus reduced to a set of matrix equations in the Landau indices, with the order of the matrices determined by the ratio of the cyclotron frequency to the width of the energy shell, and the dispersion of the energy in the third dimension:

$$\underline{G}(\mathbf{R};i\omega_\nu)=[\underline{1}+\underline{G}^0(i\omega_\nu)\underline{\Delta}(\mathbf{R})\underline{G}^0(-i\omega_\nu)\underline{\Delta}^\dagger(\mathbf{R})]^{-1}\times\underline{G}^0(i\omega_\nu)\ , \tag{14a}$$

$$\underline{F}^\dagger(\mathbf{R};i\omega_\nu)=-\underline{G}^0(-i\omega_\nu)\underline{\Delta}^\dagger(\mathbf{R})\underline{G}(\mathbf{R};i\omega_\nu)\ , \tag{14b}$$

where the underbar denotes matrices in the Landau-level indices (or partitioned spin matrices for nonzero g factors). These equations thus determine F as a function of A^P, closing the self-consistency loop of Eqs. (10) and (13) and hence also the BCS superconducting state within the constant-field approximation.

Symmetry of the lattice can be used to simplify the calculation by eliminating those values of A^P that are inconsistent with the rotational invariance of the lattice. For the square lattice, we find that all nonzero A^P's have P values of $4k+2j$ where j is determined from free-energy considerations and can take values of 0 or 1, and $k=0,1,2,\ldots$, and for the triangular lattice $P=6k+2j$,

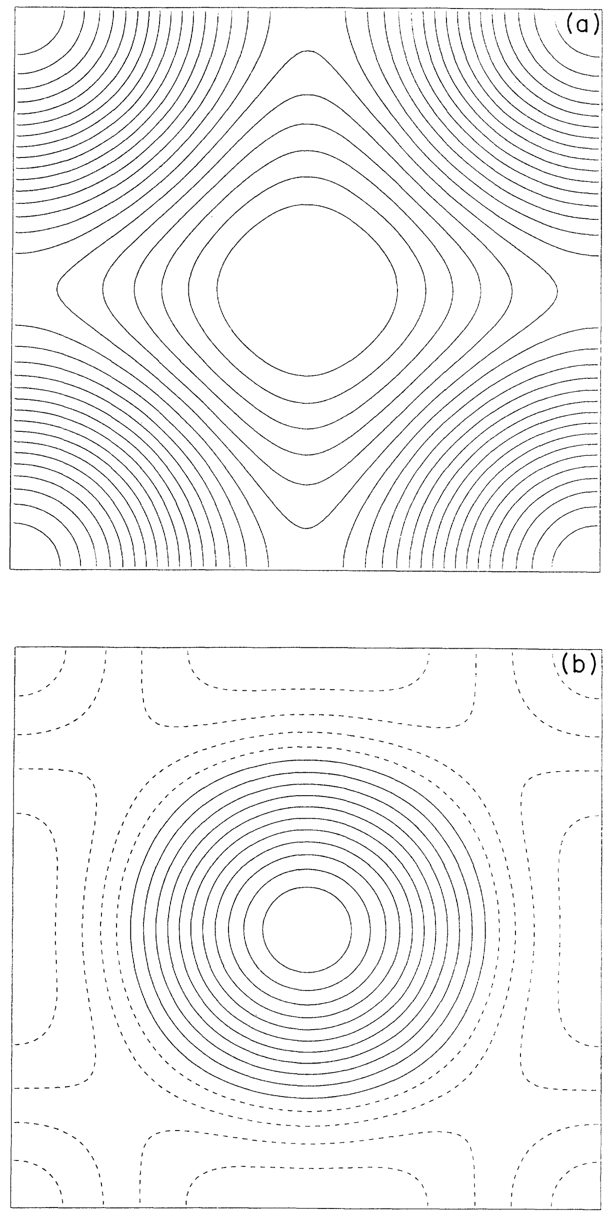

FIG. 1. Contour plot of the (a) $|\Delta^0(r)|^2$ and (b) $\mathrm{Re}[\Delta^0(r)\Delta^{4*}(r)]$ in one unit cell of the square lattice. Zeros are found at the corners. Dotted contours represent negative values.

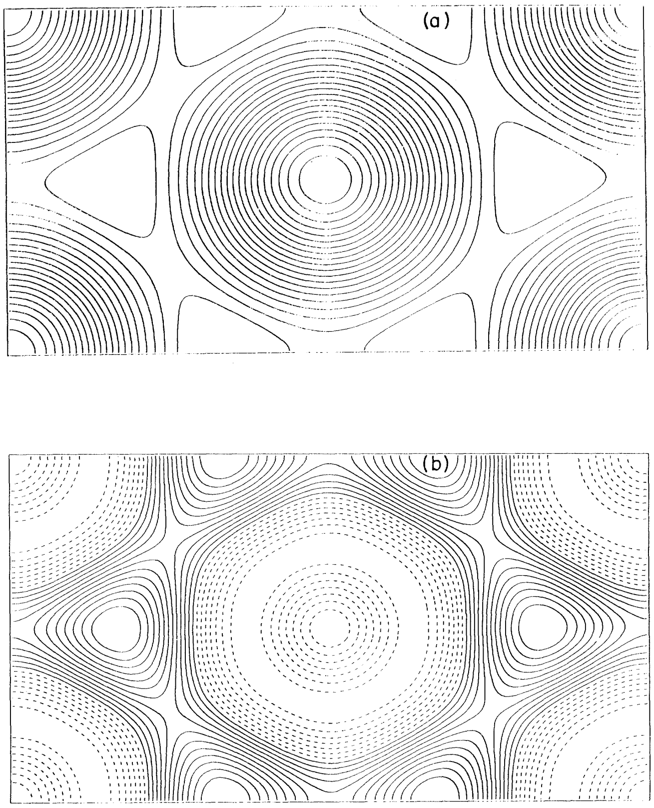

FIG. 2. Contour plot of the (a) $|\Delta^0(r)|^2$ and (b) $\mathrm{Re}[\Delta^0(r)\Delta^{6*}(r)]$ in one unit cell of the triangular lattice. Zeros are found at the corners and at the center. Dotted contours represent negative values.

where j can have values of 0, 1, or 2. (Rotational properties of the lattice are given in the Appendix). It will be shown below that the largest T_{c2} is obtained for Cooper pairing in the $P=0$ Landau index so that $j=0$ is the only physically relevant solution, in contrast to Ref. 13, where the $j=1$ solution was discussed.

The spatial form of the Abrikosov solution is identical to the $P=0$ lattice construction. However, as Cooper pairs are formed in higher Landau indices, the spatial profile of the order parameter, density of states, and current distribution etc. will differ significantly from the Abrikosov solution. As the temperature is lowered, the first deviation from the Abrikosov form of the order parameter squared is the real part of $\Delta^0(\mathbf{r})\Delta^{4*}(\mathbf{r})$ for the square lattice, and $\Delta^0(\mathbf{r})\Delta^{6*}(\mathbf{r})$ for the triangle. It is interesting to note that these terms give both positive and negative contributions to the order parameter as is illustrated in Figs. 1 and 2.

IV. DIAGONAL APPROXIMATION

As an illustration of the above procedure, we examine a simple model of an isotropic three-dimensional superconductor with the Debye energy ω_D, the zero-field Fermi energy E_f, and the zero-field critical temperature T_c taken to be $E_f=1000T_c$ and $\omega_D=100T_c$. The energy eigenvalues are $\varepsilon_N=\omega_c(N+1/2)+k_z^2/2m-\mu$, so that the states participating in the pairing are all the states with N below $N_{\max}=(\mu+\omega_D)/\omega_c-1/2$ and with momentum between $\mu-\omega_c(N+1/2)-\omega_D<k_z^2/2m<\mu-\omega_c(N+1/2)+\omega_D$ for each N. Linearization of the right-hand side of Eq. (10) in A^P gives the condition for the onset of the pairing instability at temperature T_{c2} first given in Ref. 19. Here this equation takes the form, independent of the lattice structure,

$$1=\frac{\bar{V}N(0)\omega_c}{4}\sum_{N_1N_2}(C^P_{N_1N_2})^2\int\frac{dk_z}{k_f}\frac{\tanh(\beta\varepsilon_{N_1}/2)+\tanh(\beta\varepsilon_{N_2}/2)}{2(\varepsilon_{N_1}+\varepsilon_{N_2})}\,, \tag{15}$$

where k_f is the zero-field Fermi wave vector, $N(0)=mk_f/2\pi^2$ is the zero-field density of states at the Fermi energy, and the bounds of integration on k_z are as given above. This shows that there will be a different T_{c2} for each value of P. However, only the P value that yields the highest T_{c2} is of significance since growth of the corresponding A^P will render invalid the linearization of Eq. (10) near lower-T_{c2} values. If one considers only the pairing between two electrons in one Landau level with index N, keeping only the $N_1=N_2=N$ term, the onset of the instability in the $P=0$ and $P=2N$ pairing channels would occur at the same temperature[13] $[C^0_{NN}=(-1)^N C^{2N}_{NN}]$. However, since an electron can pair with other electrons within the attractive energy shell, other terms in the above equation will lead to more electrons pairing in the $P=0$ channel than in any given $2N$ channel. Therefore, the $P=0$ pairing channel will have the largest T_{c2}. A calculation of T_{c2} shows the appearance of the superconducting state at $\omega_c/E_f=0.750$, 0.422, 0.295, and 0.227 with 0.004 respectively. In Fig. 3 we plot the values of T_{c2} for $N_{\max}=2,3,4$, along with the chemical potential, illustrating that the T_{c2} peaks appear each time the Fermi level crosses a Landau level. We will refer to these field values by their $N_{\max}$ values, since the major contribution to pairing—at high fields where there is only a single peak of the density of states in the pairing shell—comes from the $N_{\max}$ states.

We now calculate the first few nonzero A^P's for some of these magnetic-field values at which the superconducting state appears. For calculational simplicity we ignore all inter-Landau-level pairing, which is a good approximation in high fields.[14] In fact, we find no discernible difference between the results shown in Fig. 3 and those

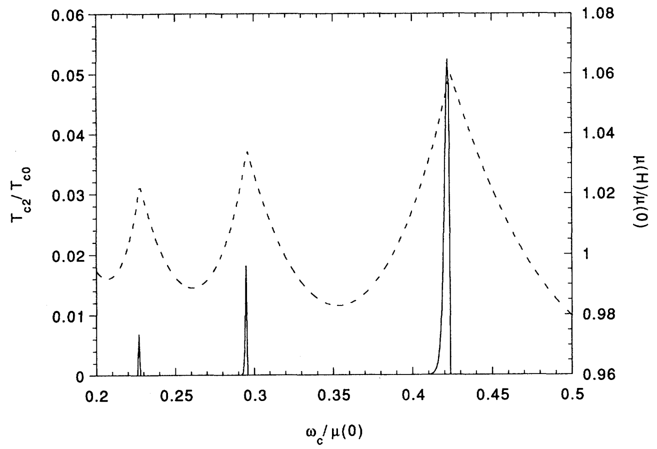

FIG. 3. Plot of T_{c2} vs magnetic field showing the $N_{max}=2,3,4$ peaks. Also shown (dotted line) is the chemical potential.

obtained with the diagonal approximation. For lower-field values, the number of off-diagonal terms increases rapidly, rendering the diagonal approximation invalid. The matrices in Eqs. (14a), (14b) are diagonal, resulting in the following self-consistent equation for A^P:

$$A^P=\frac{\overline{V}N(0)\omega_c}{4}\sum_N C_{NN}^P\int\frac{d^2R}{a_y}\phi_{2N-P}^{\rm cm}(\mathbf{R})\times\Delta_N^\dagger(\mathbf{R})T_N(\mathbf{R})\ , \qquad (16a)$$

with

$$T_N(\mathbf{R})=\int\frac{dk_z}{k_f}\frac{\tanh[\beta E_N(\mathbf{R})/2]}{2E_N(\mathbf{R})}\ , \qquad (16b)$$

where E_N are the quasiparticle energies given by

$$E_N(\mathbf{R})=[\varepsilon_N^2+|\Delta_N(\mathbf{R})|^2]^{1/2}\ , \qquad (17)$$

and with Δ given in terms of A^P by Eq. (13). The area of integration covers one period in the Y direction and is infinite in the X direction.

Near T_{c2}, A^P can be calculated by expanding T_N in the above expressions (16a) and (16b) to second order in A^P. This facilitates an analytic evaluation of the R integral in Eq. (16a). We display these results in Figs. 4 and 5 showing the growth of $A^Pa_y^{1/2}$ as the temperature is decreased below T_{c2} for $N_{max}=1,2,3,4$ for the two lattice structures. The factor of $a_y^{1/2}$ is convenient because the free energy calculation from the GL expansion of the free energy to order $|\Delta|^2$ is

$$\mathcal{F}_s-\mathcal{F}_n\propto a_y\sum_P[A+(2P+1)C/l^2]|A^P|^2\ , \qquad (18)$$

where C is the coefficient of the derivatives of Δ, $A<0$, $C>0$, and $A+C/l^2<0$ for a type-II superconductor.[4] In this way it is easy to see that the triangular lattice has a lower free energy than the square.

For $N_{max}=1$, the electrons would energetically be able to form pairs up to $P=2$. However, from the symmetry restrictions mentioned above, neither $P=1$ nor $P=2$ is allowed in either lattice so that only A^0 is nonzero. As the field is decreased to $N_{max}=2$, electrons can pair in the $P=4$ channel, and then A^4 becomes nonzero for the square. At $N_{max}=3$, no new pairing channels are allowed in the square lattice, but $P=6$ now appears in the triangular lattice. These results are shown in Figs. 4 and 5. It is interesting to note that the relative strength of the $P=4$ amplitude is smaller for $N_{max}=3$ than for $N_{max}=2$. This is because the N_{max} pairing in $P=2N_{max}$ is always stronger than for P between zero and $2N_{max}$, due to the overlap integrals ($|C_{NN}^0|=|C_{NN}^{2N}|>|C_{NN}^P|$ for $0<P<2N$).

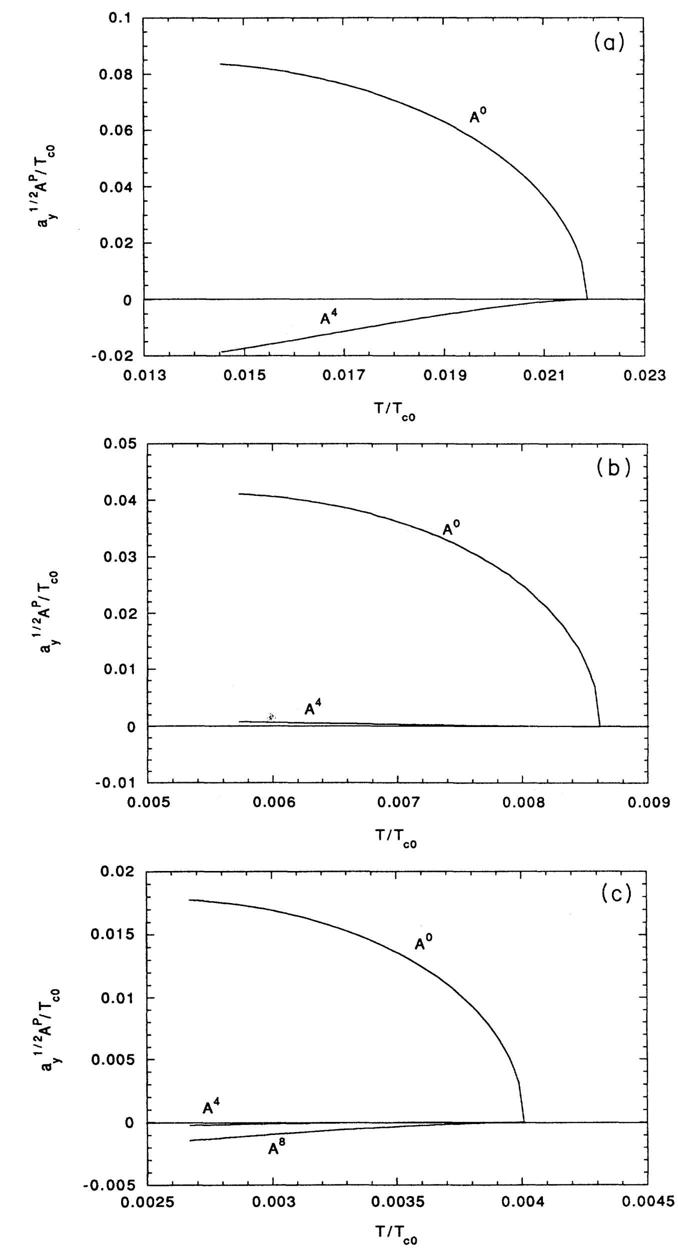

FIG. 4. A^P vs T for the square lattice with $N_{max}=$ (a) 2, (b) 3, (c), 4.

This is illustrated even more clearly when the field values reach $N_{max}=4$. Here we see that $P=8$ pairing is not only possible in the square lattice, but has a greater amplitude than for $P=4$ pairing. It can also be seen that there is more pairing of electrons in higher Cooper pair Landau states for the square lattice than for the triangular lattice at the same field strength.

As the field is decreased further, higher-N level participate in the pairing. At low enough fields, there are multiple levels lying within the pairing shell and the pairing is no longer dominated by electrons within a single level. The numbers of possible interlevel pairings and possible intralevel pairings increase as N^2 and N, respectively. The diagonal approximation thus becomes increasingly inappropriate for such low fields. Eventually we pass into a semiclassical regime where large-N values dominate and a different scheme is necessary to handle the N sums in the above equations. This limit is expected to approach the original Abrikosov solution in the semiclassical approximation.[23] The details of this will be discussed in a separate publication.

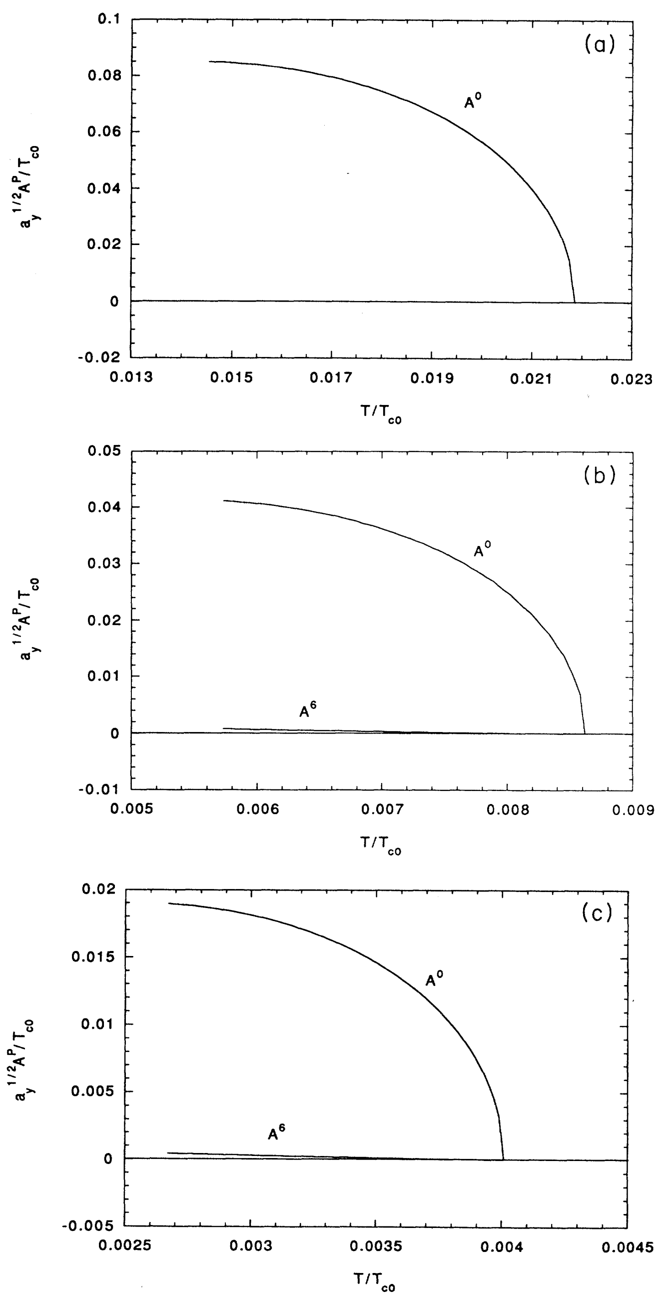

FIG. 5. A^P vs T for the triangular lattice with $N_{max}=$ (a) 2, (b) 3, (c) 4.

V. CONCLUSION

We have presented a theory of vortex solutions of the Gorkov equations in strong magnetic fields. We have solved these equations in a simplified model to illustrate the appearance of Cooper pairing in higher-Landau indices ($A^P, P\neq 0$), showing how the profile of the order parameter differs from the Abrikosov solution. This formulation provides an insight into the microscopic origin of the vortex structure as being due to correlations among the degenerate states of the single-particle Landau states.

We have also shown that the set of amplitudes, $\{A^P\}$, determine fully both the one-particle Green's function and the anomalous Green's function from which quantities of interest such as the local density of states at any energy (useful in interpreting STM data) and various response functions can be calculated. In the present work we have limited ourselves to a constant-field regime near T_{c2}; to go beyond this regime, the induced magnetic field must also be calculated self-consistently along with the amplitudes. While this requires a more involved calculation with different forms for the Green's functions, the form of the order parameter remains the same with only the values of the pairing amplitudes being affected.

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APPENDIX

In this appendix we discuss the rotational-translational properties of the Landau states which generate the lattice. The symmetric gauge $\mathbf{A}(\mathbf{r})=\mathbf{H}\times\mathbf{r}/2$ is of clear advantage when treating rotations since it transforms as a vector. The wave functions in the rotated frame have the form of Eq. (4b) with x' and y' expressed in this frame. The transformation matrix is defined as

$$\langle NX|D(\theta)|N'X'\rangle=\int\frac{d^2r}{2\pi l^2}\psi^*_{NX}(\mathbf{r})D(\theta)\psi_{N'X'}(\mathbf{r})\ , \qquad (A1)$$

where the operator $D(\theta)$ rotates the vector $\mathbf{r}$ through an angle θ about the magnetic-field direction

$$D(\theta)=\exp(i\theta L_z)\ , \qquad (A2)$$

with the generator of rotations in the symmetric gauge $L_z = xp_y - yp_x$ given by

$$\langle NX|D(\theta)|N'X'\rangle = \delta_{N,N'}\frac{[\pi(1-e^{2i\theta})]^{1/2}}{2\pi l|\sin\theta|}e^{iN\theta} \times \exp\left[i\frac{(X^2+X'^2)\cos\theta - 2XX'}{2l^2\sin\theta}\right] . \tag{A3}$$

Similarly, the magnetic translation operator is given by

$$T(\mathbf{a}) = \exp\{i[\mathbf{p}+(e/c)\mathbf{A}(\mathbf{r})]\cdot\mathbf{a}\} , \tag{A4}$$

with the corresponding transformation matrix

$$\langle NX|T(\mathbf{a})|N'X'\rangle = \delta_{N,N'}\exp(ia_x a_y/2l^2) \times \exp(-iX'a_y/l^2)\delta(X-X'+a_x) . \tag{A5}$$

Point-group operations about the zeros of the order parameter will leave its absolute square invariant. It can be shown that all even P terms have zeros in the same place as the $P=0$ term, and that all A^P for odd P can be eliminated by inversion symmetry. It should be emphasized that the use of symmetry here introduces no new assumptions. Direct application of Eq. (16) will produce the same results without *a priori* use of rotational symmetry arguments.

Zeros of $\Delta(\mathbf{r})$ for the square lattice fall on all points equivalent to the origin. Application of $D(\theta)$ directly to Eq. (9) [with l in Eq. (A3) replaced by $l/2^{1/2}$] with the requirement $|\Delta(\mathbf{r})|^2 = |D(\theta)\Delta(\mathbf{r})|^2$ for $\theta=\pi/2$ or $3\pi/2$, leads to $\exp[i(P-P')\theta]=1$. Therefore the only nonzero values of A^P must have P values differing by a factor of 4.

The zeros of $\Delta(\mathbf{r})$ for the triangular lattice are found at $\mathbf{r}=(a_x/4, a_y/4)$ and $(3a_x/4, 3a_y/4)$. Therefore the symmetry operations of the lattice are a combination of a translation of the origin to one of the zeros, rotation through an integral multiple of $\pi/6$, and a translation to return the origin to its original location: $|\Delta(\mathbf{r})|^2 = |T^{-1}D(\theta)T\Delta(\mathbf{r})|^2$. In this case, the only nonzero values of A^P must have P values differing by a factor of 6.

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