Wannier-function approach to phase transitions in superconducting films

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We describe a method for treating fluctuations in two-dimensional superconducting films in zero magnetic field. The method involves expanding the order parameter $\psi(x,y)$ in empty-lattice Wannier functions of a fictitious square lattice. Despite the discrete basis, the order parameter is *continuous* and has no unphysical pinning. The thermodynamics of the model is a function of a single variable analogous to the Josephson coupling in granular superconductors. We estimate the Kosterlitz-Thouless (KT) transition temperature T_c of the model by Monte Carlo techniques. If amplitude fluctuations are neglected, the model reduces to a partially frustrated XY Hamiltonian, even in zero magnetic field. With amplitude fluctuations, T_c is further reduced, the Coulomb-gas scaling hypothesis of Minnhagen is automatically satisfied, and the jump in superfluid density at the transition may possibly be nonuniversal. Snapshots of $\psi(x,y)$ near T_c reveal the rapid development of pairs of oppositely charged vortices, accompanied by zeros of the order parameter, and, above T_c, by unpaired vortices, in agreement with the original KT picture. The extension of this approach to layered three-dimensional superconductors is briefly discussed.

I. INTRODUCTION

The so called XY or planar model has an unusual "Kosterlitz-Thouless" (KT) phase transition in two dimensions (2D).[1] Instead of a magnetization which vanishes continuously according to a power law at the transition temperature T_c, the low-temperature phase is actually a state of zero magnetization. Below T_c, the excitations consist of bound vortex-antivortex pairs. Above T_c, some of the vortex pairs unbind to produce a finite density of free vortices. Precisely at T_c, the helicity modulus γ has a universal jump of magnitude $\gamma(T_c)/k_B T_c = 2/\pi$.[2]

The KT theory has been applied with particular success to thin superconducting films. In these materials, the universal jump in γ has numerous experimental consequences,[3–6] such as a power-law current-voltage characteristic below T_c (Ref. 5) and a universal scaling of resistivity with temperature above T_c.[4–6] This behavior has been observed in both thin superconducting films[7–10] and superconducting arrays. Even bulk high-T_c materials such as $YBa_2Cu_3O_{7-\delta}$ (YBCO) or $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) show some experimental evidence for KT-like behavior,[11–13] primarily in the power-law current-voltage characteristics and resistivity scaling. This behavior probably arises from the highly anisotropic layered structure of these materials.

The XY model is not entirely suitable for describing the KT transition in superconducting films. One problem is that the XY spins are discrete variables on a lattice, whereas the order parameter $\psi(x,y)$ in a superconducting film is continuous. This difference may be irrelevant sufficiently near T_c, where the properties are universal. Nevertheless, one cannot easily compute from the XY model many important *nonuniversal* properties, such as the continuous spatial distribution of the order parameter in a given configuration or T_c itself.

In this paper we describe a simple way to remedy this problem, while still retaining the convenience of a lattice-based calculation. We expand the other parameter $\psi(\mathbf{r})$ in a complete set of *Wannier functions* on a square lattice. The Wannier functions we choose are associated with an empty-lattice (i.e., a plane-wave) basis. We truncate the expansion, by including only Wannier functions drawn from the *lowest band.* This truncation is roughly analogous to the so-called lowest Landau level (LLL) approximation which has been successfully used to treat 2D superconducting films in a magnetic field.[14]

When the truncated expansion is substituted into a Ginzburg-Landau free-energy functional, we obtain a discrete functional which closely resembles the XY Hamiltonian. But our functional has interactions (both "ferromagnetic" and "antiferromagnetic") beyond the nearest-neighbor shell, and includes amplitude as well as phase fluctuations. The model can readily be treated by Monte Carlo (MC) methods, and leads to KT transition temperature closely related to other measurable properties of the film. Furthermore, if the lattice constant is appropriately chosen, the model automatically satisfies the Coulomb-gas scaling hypothesis of Minnhagen.[15]

The calculated order parameter can be displayed in real space. The vortex-antivortex pairs predicted by the KT theory appear directly as pairs of zeroes of the order parameter. The number of these increases sharply as the temperature approaches T_c from below, as expected. The positions of these excitations correspond well to those predicted, on the basis of a lattice picture, by Tobochnik and Chester.[16] However, they are not confined to the lattice sites but can occur at any point in the film.

We turn now to the body of the paper. Our formalism is outlined in Sec. II. Numerical MC results are presented in Sec. III. A brief discussion follows in Sec. IV.

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II. FORMALISM

We consider a two-dimensional superconducting film, of thickness L_z. We will assume that the film is in the extreme-type-II limit (Ginzburg-Landau parameter $\kappa \gg 1$, where $\kappa \equiv \lambda/\xi$ is the ratio of the mean-field penetration depth λ to the mean-field coherence length ξ), so that the magnetic field induced by the screening currents can be neglected. If there is no applied magnetic field, the film is described by a Ginzburg-Landau free-energy functional

$$F = L_z \int d^2r \left\{ \alpha(T)|\psi(\mathbf{r})|^2 + \frac{\beta}{2}|\psi(\mathbf{r})|^4 + \frac{\hbar^2}{2m^*}|\nabla\psi(\mathbf{r})|^2 \right\} . \tag{1}$$

Here, $\alpha(T)=\alpha'(T-T_{c0})$, T_{c0} is the mean-field transition temperature in zero field, $\psi(\mathbf{r})$ is the complex scalar order parameter, $\mathbf{r}\equiv(x,y)$, and α', β, and m^* are material-dependent constants. We assume that ψ is independent of z.

To calculate the thermodynamics, we can expand $\psi(\mathbf{r})$ in any desired complete set of basis functions. We will choose a set of *Wannier functions* corresponding to an empty-lattice band structure on a square lattice. With this choice, we can calculate the thermodynamic properties by a straightforward MC procedure.

In any 2D periodic solid, a normalized Wannier function $u_{n\mathbf{R}}(\mathbf{r})$ is defined in terms of the corresponding set of Bloch functions $\Phi_{n\mathbf{k}}(\mathbf{r})$ by

$$\Phi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} \exp(i\mathbf{k}\cdot\mathbf{R}) u_{n\mathbf{R}}(\mathbf{r}) , \tag{2}$$

where n and $\mathbf{R}$ are the band and site indices. The Wannier functions are chosen to be orthogonal, and are normalized so that the coefficients are size independent:

$$\int d^2r\, u^*_{n\mathbf{R}}(\mathbf{r}) u_{n'\mathbf{R}'}(\mathbf{r}) = A_0 \delta_{nn'} \delta_{\mathbf{R}\mathbf{R}'} , \tag{3}$$

where A_0 is the area of the Bravais lattice unit cell.

We will develop our basis from empty-lattice Bloch functions, i.e., plane waves whose energy spectrum is folded back into the first Brillouin zone of an appropriate Bravais lattice:

$$\Phi_{n\mathbf{k}}(\mathbf{r}) = \exp[i(\mathbf{k}+\mathbf{K}_n)\cdot\mathbf{r}] , \tag{4}$$

where $\mathbf{K}_n$ is the nth reciprocal-lattice vector. We choose a square Bravais lattice of lattice constant a to be specified later. The normalized Wannier function for the *lowest* ($\mathbf{K}_0=0$) band is

$$u_{0\mathbf{R}}(\mathbf{r}) = u_{00}(\mathbf{r}-\mathbf{R}) , \tag{5}$$

where

$$u_{00}(\mathbf{r}) = f\left[\frac{x}{a}\right] f\left[\frac{y}{a}\right] \tag{6}$$

and

$$f(u) = \frac{\sin(\pi u)}{\pi u} . \tag{7}$$

The next step is to expand the order parameter $\psi(\mathbf{r})$ in Wannier functions from the lowest band. Including only the lowest band imposes a large-k cutoff in the fluctuations. This is certainly reasonable within the Ginzburg-Landau formalism, which describes only the dominant long-wavelength fluctuations in $\psi(\mathbf{r})$. The expansion is

$$\psi(\mathbf{r}) = \sum_{\mathbf{R}} C_{\mathbf{R}} u_{0\mathbf{R}}(\mathbf{r}) . \tag{8}$$

When this is substituted into the free-energy functional (1), we obtain $F=F^{(2)}+F^{(4)}$, where

$$F^{(2)} = L_z a^2 \sum_{\mathbf{R}} \alpha(T)|C_{\mathbf{R}}|^2 + L_z \frac{\hbar^2}{2m^*} \sum_{\mathbf{R},\mathbf{R}'} C_{\mathbf{R}} C^*_{\mathbf{R}'} U_{\mathbf{R},\mathbf{R}'} \tag{9}$$

and

$$F^{(4)} = L_z \frac{\beta}{2} a^2 \sum_{\mathbf{R},\mathbf{R}',\mathbf{R}'',\mathbf{R}'''} C_{\mathbf{R}} C_{\mathbf{R}'} C^*_{\mathbf{R}''} C^*_{\mathbf{R}'''} M_{\mathbf{R},\mathbf{R}',\mathbf{R}'',\mathbf{R}'''} . \tag{10}$$

Here,

$$U_{\mathbf{R},\mathbf{R}'} = \int d^2r\, \nabla u_{0\mathbf{R}}(\mathbf{r})\cdot\nabla u^*_{0\mathbf{R}'}(\mathbf{r}) \tag{11}$$

and

$$M_{\mathbf{R},\mathbf{R}',\mathbf{R}'',\mathbf{R}'''} = \frac{1}{a^2} \int d^2r\, u_{0\mathbf{R}}(\mathbf{r}) u_{0\mathbf{R}'}(\mathbf{r}) u^*_{0\mathbf{R}''}(\mathbf{r}) u^*_{0\mathbf{R}'''}(\mathbf{r}) . \tag{12}$$

For a square lattice, using the translational symmetry of the free-energy functional, we can express the dimensionless coefficients in the form

$$U_{\mathbf{R},\mathbf{R}'} = U_{m-m',n-n'} \tag{13}$$

and

$$M_{\mathbf{R},\mathbf{R}',\mathbf{R}'',\mathbf{R}'''} = V_{m'-m,m''-m,m'''-m} V_{n'-n,n''-n,n'''-n} , \tag{14}$$

where we have written $\mathbf{R}=a(m\hat{\mathbf{x}}+n\hat{\mathbf{y}})$. The coefficients U can be evaluated analytically, with the results

$$U_{0,0} = \frac{2\pi^2}{3} \tag{15}$$

and

$$U_{m,n} = 2\left[\frac{(-1)^m}{m^2}\delta_{n,0} + \frac{(-1)^n}{n^2}\delta m,0\right] , \tag{16}$$

otherwise. The first few values are $U_{0,1}=-2$, $U_{0,2}=+\frac{1}{2}$, $U_{0,3}=-\frac{2}{9}$, and $U_{0,4}=+\frac{1}{8}$. Similarly, we find

$$V_{m_1,m_2,m_3} = \int dx\, f(x) f(x-m_1) f(x-m_2) f(x-m_3) . \tag{17}$$

The first few V coefficients evaluated numerically are $V_{0,0,0}=+0.6666\ldots$, $V_{0,1,1}=+0.101\,32$,

$$V_{0,0,1}=+0.050\,66, \quad V_{0,-1,1}=-0.050\,66 ,$$

$$V_{1,1,2}=+0.050\,66, \quad V_{0,1,2}=-0.025\,33 ,$$

$$V_{0,0,2}=-0.012\,66\ .$$

Because of numerous index symmetries (e.g., $V_{i,j,k}=V_{i,k,j}=V_{j,i,k}=V_{j,k,i}=V_{k,i,j}=V_{k,j,i}$ and $V_{i,j,k}=V_{-i,-j,-k}=V_{i,i-j,i-k}=V_{j,j-i,j-k}=V_{k,k-i,k-j}$), many coefficients can be found from these few integrals.

Using Eqs. (9) and (10), we can rewrite F as

$$F=L_z\frac{\hbar^2}{2m^*}\frac{|\alpha(T)|}{\beta}\left[-\frac{a^2}{\xi^2(T)}\sum_{m,n}|c_{m,n}|^2+\sum_{\substack{m,m'\\n,n'}}c_{m,n}c^*_{m',n'}U_{m-m',n-n'}\right.$$
$$\left.+\frac{1}{2}\frac{a^2}{\xi^2(T)}\sum_{\substack{m\ldots m'''\\n\ldots n'''}}c_{m,n}c_{m',n'}c^*_{m'',n''}c^*_{m''',n'''}V_{m'-m,m''-m,m'''-m}V_{n'-n,n''-n,n'''-n}\right]\ . \tag{18}$$

Here, $c_{m,n}=C_{m,n}/\psi_0$, $\psi_0=\sqrt{-\alpha(T)/\beta}$ is the mean-field order parameter, and $\xi(T)$ is the mean-field correlation length, defined by

$$\xi^2(T)=\frac{\hbar^2}{2m^*|\alpha(T)|}\ . \tag{19}$$

$\xi(T)$ is the only length scale of the problem, and sets the natural ultraviolet cutoff $k_{\max}\sim 1/\xi(T)$ for excitations in the system. Given F, the Helmholtz free-energy density $\mathcal{F}$ is obtained from the expression

$$\mathcal{F}=-\frac{k_BT}{(Na)^2L_z}\times\ln\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\Pi_{\mathbf{R}}dc_{\mathbf{R}1}dc_{\mathbf{R}2}\exp(-F/k_BT)\ , \tag{20}$$

where Na is the length of one side of a square sample, and we have written $c_{\mathbf{R}}=c_{\mathbf{R}1}+ic_{\mathbf{R}2}$.

The present formalism has a number of appealing features which make it especially suitable for treating superconducting films. First, the spatially uniform ground state (i.e., $\psi=\psi_0=$const) has a simple expression in terms of the lowest band of this Wannier basis, namely, $c_{\mathbf{R}}=1$ for all $\mathbf{R}$. Second, the free energies of any states connected by a uniform translation, i.e., $\psi(\mathbf{r})$ and $\psi(\mathbf{r}-\mathbf{r}_0)$, are *equal,* even if $\mathbf{r}_0$ is *not a lattice vector.* Thus, even though the model is based on a discrete Bravais lattice, it introduces *no artificial pinning.* The model is translationally invariant for any choice of lattice constant, and even though ψ is expanded in Wannier states drawn from only the *lowest* Bloch band. The translational invariance is not guaranteed, however, if $F^{(2)}$ and $F^{(4)}$ are approximated in some way. Nevertheless, in our calculations, we see no evidence of unphysical pinning provided that we include amplitude fluctuations in our approximation. This point is discussed further below.

The form (18) for the free energy suggests a natural, temperature-dependent choice for the lattice constant,[5] namely, $a=\xi(T)$. With this choice, all fluctuations of wavelength longer than $\xi(T)$ are still included. In addition, the entire free energy depends on a single (temperature-dependent) coupling constant which we write as

$$J\equiv 4L_z\frac{\hbar^2}{2m^*}\frac{|\alpha(T)|}{\beta}=\frac{\Phi_0^2}{8\pi^3}\frac{L_z}{\lambda^2(T)}\ , \tag{21}$$

where $\Phi_0=hc/2e$ is the flux quantum and $\lambda(T)$ is the mean-field penetration depth. Alternatively, J can be expressed in terms of experimentally accessible quantities, as in Ref. 17. The result is

$$J=L_z\Phi_0\left|\frac{dH_{c2}}{dT}\right|_{T=T_{c0}}\frac{T_{c0}-T}{4\pi^2\kappa^2}\ . \tag{22}$$

Hence, the phase transition, in this approximation, is entirely governed by the dimensionless temperature $\mathcal{T}=k_BT/J$. An analogous reduction occurs in the scaling theory of the Coulomb-gas transition in the Ginzburg-Landau approximation.[15] In that model, all dimensionless quantities are expressed in terms of a dimensionless Coulomb-gas temperature T^{CG}. The two dimensionless temperatures are simply related by $\mathcal{T}=\pi T^{CG}$.

The phase-dependent part of $F^{(2)}$ can be rewritten in the form

$$\tfrac{1}{2}\textstyle\sum_{\mathbf{R}\neq\mathbf{R}'}J_{\mathbf{R},\mathbf{R}'}\cos(\theta_{\mathbf{R}}-\theta_{\mathbf{R}'})\ ,$$

where the $J_{\mathbf{R},\mathbf{R}'}$'s are temperature-dependent coefficients of either sign and $c_{\mathbf{R}}\equiv|c_{\mathbf{R}}|\exp(i\theta_{\mathbf{R}})$. Thus, *F formally* resembles a network of Josephson-coupled coherent regions. However, this picture differs in several ways from previous "granular" pictures of homogeneous films.[18] For example, the coupling alternates between ferromagnetic and antiferromagnetic, rendering the ground state partially frustrated even without an applied magnetic field. In addition, the coupling constant is temperature dependent. Most important, the resulting order parameter $\psi(\mathbf{r})$ varies continuously in space, without pinning.

In actual calculations, we have approximated $F^{(4)}$ by a simple *diagonal* form with no phase dependence:

$$F^{(4)}=\frac{J}{8}\sum_{\mathbf{R}}|c_{\mathbf{R}}|^4\ . \tag{23}$$

We chose this form after observing that the diagonal terms of the original expansion (10) have the largest coefficients, and that the phase dependence of $F^{(4)}$ is in general weak in comparison to that of $F^{(2)}$. It can be shown that the approximate form (23) still leaves the free

energy translationally invariant provided that only Fourier modes $\Phi_{0\mathbf{k}}$ near the center of the first Brillouin zone are excited. Furthermore, (23) gives the ground-state energy *exactly,* and gives excited-states energy to within 2%. We have checked this error estimate by comparing the approximate diagonal value of $F^{(4)}$ after each MC run to the exact result obtained by numerical integration of $|\psi|^4$. Thus, numerically, the diagonal form is really an excellent approximation, although, analytically, the argument for writing it down is somewhat arbitrary.

We describe most of our results in terms of the *helicity modulus tensor* γ_{ij}. This is defined by the relation

$$\gamma_{ij}=\left[\frac{\partial^2\mathcal{F}}{\partial A_i'\partial A_j'}\right]_{\mathbf{A}'=0}, \tag{24}$$

where $\mathbf{A}'$ is an added constant vector potential imposed in the presence of periodic boundary conditions. To express γ in terms of the amplitudes $c_{\mathbf{R}}$, we incorporate a gauge-invariant phase difference into the free-energy functional (18). The phase-dependent part of (18) takes the form

$$\frac{J}{4}\sum_{\mathbf{R}\neq\mathbf{R}'}|c_{\mathbf{R}}||c_{\mathbf{R}'}|\cos\left[\theta_{\mathbf{R}}-\theta_{\mathbf{R}'}-\frac{2\pi}{\Phi_0}\mathbf{A}'\cdot(\mathbf{R}-\mathbf{R}')\right]U_{\mathbf{R},\mathbf{R}'}\ . \tag{25}$$

By direct differentiation (using the mass normalization $2e\hbar/m^*c=1$ and taking $\mathbf{A}'=A'\hat{\mathbf{x}}$), we find that

$$\gamma_{xx}=\frac{1}{N^2}\left[\frac{4\pi\psi_0^2}{\Phi_0}\right]\left[\sum_{p=1}^{\infty}(-1)^{p+1}\left\langle\sum_{m,n}\Re\{c_{m,n}c_{m+p,n}^*\}\right\rangle-\frac{1}{\mathcal{T}}\left\langle\left[\sum_{p=1}^{\infty}\frac{(-1)^p}{p}\sum_{m,n}\Im\{c_{m,n}c_{m+p,n}^*\}\right]^2\right\rangle\right], \tag{26}$$

where $\langle\cdots\rangle$ denotes a thermal average in the canonical ensemble. In the ground state (i.e., $c_{\mathbf{R}}=1$), γ_{xx} is equal to its mean-field value $\gamma_{xx}^{MF}=4\pi\psi_0^2/\Phi_0$. In this isotropic system, $\gamma_{xx}=\gamma_{yy}$.

III. RESULTS

We have considered several different approximations to the model (18), as well as several different sample sizes. In the simplest approximation (model I), we neglect amplitude fluctuations (i.e., we replace $|c_{\mathbf{R}}|$ by its mean-field value), and we also include only nearest-neighbor coupling. Equation (18) then reduces to the well-known 2D ferromagnetic XY model with nearest-neighbor couplings only. This model has a KT transition at $\mathcal{T}_c=0.89$.[16] The next step up in complexity is to include further neighbors in the XY coupling (model II), thus including both ferromagnetic and antiferromagnetic interactions, while still neglecting amplitude fluctuations in the coefficients $c_{\mathbf{R}}$. Finally, the most complete version of the model (model III) includes both amplitude fluctuations in the diagonal approximation [Eq. (23)] and many shells of neighbors.

Note that in both models I and II, $|\psi(\mathbf{R})|=\psi_0$, the mean-field value, for all $\mathbf{R}$. Likewise, the spatial average $|\psi(\mathbf{r})|^2=\psi_0^2$. In both cases, however, the density $|\psi(\mathbf{r})|^2$ in any given configuration is a function of $\mathbf{r}$. But both models also produce an unphysical pinning of thermally excited vortices. Specifically, the vortices must avoid the square mesh of empty lattice sites $\{\mathbf{R}\}$. The reason is that $|\psi(\mathbf{R})|=\psi_0$ in this approximation, whereas the order parameter must vanish at a vortex core. This unphysical pinning would be completely absent in model III if the phase dependence of $F^{(4)}$ were fully included.

To carry out our calculations, we have used the standard Metropolis algorithm, starting from the ground state, discarding the first 2500–5000 passes for equilibration and retaining the next 25 000 passes for averaging (except for our calculations on a 64×64 system, which were averaged using 15 000 passes). For models II and III, we included all neighbors through the seventh shell in the Hamiltonian.

Figure 1 shows the helicity modulus $\gamma\equiv\frac{1}{2}(\gamma_{xx}+\gamma_{yy})$ as obtained from this simulation. The error bars correspond to the rms deviation of running averages taken over 5000 passes. Clearly, the KT transition temperature T_c is substantially reduced in model II relative to model I. This is the result of the partial frustration in model II. In both cases, γ has a linear temperature dependence arising from spin waves.[19] The low-temperature derivative $|d\gamma(T)/dT|$ is larger for model II than for model I because the spin-wave modes are softer in this case. T_c is diminished yet further in model III, and $|d\gamma(T)/dT|$ is further increased at low temperatures, presumably because of the additional *density wave* degrees of freedom. In models I and II, γ exhibits the expected universal jump of $(2k_BT_c/\pi)$ at T_c. The jump may be larger than its universal value in model III. This point is discussed further below.

The additional decrease in T_c in model III can possibly be understood from the following argument: The KT transition arises from the unbinding of thermally excited vortex-antivortex pairs, which requires a certain rearrangement of order-parameter phases. The energy required for this thermally activated process is reduced in model III, because the space-averaged amplitude $\overline{|\psi|}$ is smaller than its mean-field value when amplitude fluctuations are included. Such a reduction is expected from the form of the second term in $F^{(2)}$, and, indeed, was observed in our simulations. Since these pair excitations are responsible for the phase transition, the amplitude reduction drives down T_c.

The transition in model III occurs at $\mathcal{T}_c\approx0.36$ (in our diagonal approximation). From this result, and Eq. (22),

we can predict T_c for any 2D superconductor in zero magnetic field. As an example, consider a monolayer of YBCO, taking[21] $L_z = 11.7$ Å (the interlayer spacing), $T_{c0} = 90$ K,

$$|dH_{c2}/dT|_{T=T_{c0}} = 3.2 \times 10^4 \text{ Oe K}^{-1} ,$$

and $\kappa \approx 100$. Then Eq. (22) and the above estimate for $\mathcal{T}_c$ give $T_c \approx 75$ K. This value is well below the observed transition in bulk samples, where typically T_c lies 2–3 K below T_{c0}. Presumably, interlayer coupling will increase T_c towards the observed value by making the system more three dimensional (3D).

We can also compare our MC result for T_c to a simple estimate due to Beasley, Mooij, and Orlando.[3] These authors start from the relation

$$(\hbar/m^*)^2 n_s(T_c)/(k_B T_c) = 2/\pi ,$$

where $n_s(T)$ is the 2D superfluid density. If we now substitute for n_s its mean-field value

$$n_s = m^* L_z \psi_0^2 = m^* L_z |\alpha(T)|/\beta ,$$

the prediction of Ref. 3 reduces, in our notation, to $\mathcal{T}_c = \pi/4 \simeq 0.785$. This temperature, marked with an arrow in Fig. 1, agrees well with the result from our model II, which makes an assumption rather similar to Ref. 3,

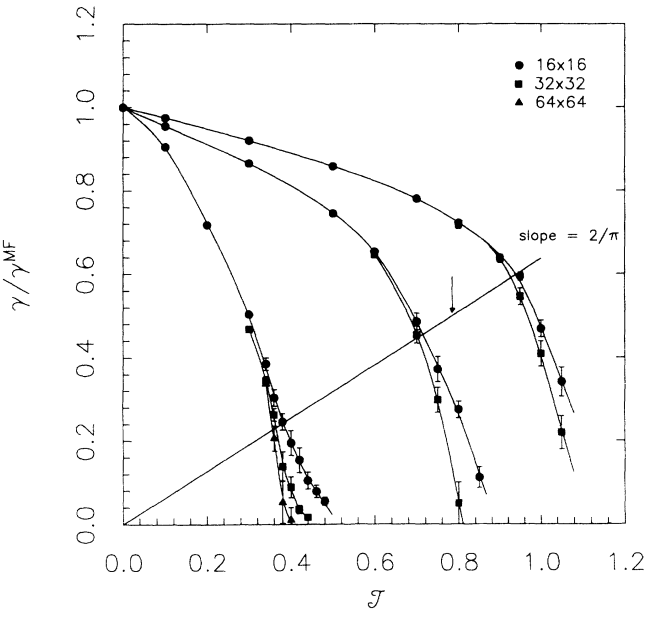

FIG. 1. Helicity modulus $\gamma \equiv \frac{1}{2}(\gamma_{xx} + \gamma_{yy})$, in units of $4\pi\psi_0^2/\Phi_0$, plotted as a function of reduced temperature $\mathcal{T}$ for various system sizes. The upper curve denotes behavior of our model I, equivalent to a classical nearest-neighbor ferromagnetic XY model on a square lattice (Ref. 20). The middle curve represents our model II, corresponding to a partially frustrated XY model with no amplitude fluctuations. The lower curve corresponds to our model III, and includes both phase and amplitude fluctuations. The solid curve of slope $2/\pi$ denotes the expected universal jump in $\gamma(T_c)/k_B T_c$ at a KT transition. Different lattice sizes are indicated in the legends to the Figure. The arrow denotes a simple estimate of $\mathcal{T}_c$ due to Ref. 3.

namely, that $\overline{|\psi(\mathbf{r})|^2}$ is a nonfluctuating quantity equal to its mean-field value ψ_0^2. In general, however, the critical temperature of Ref. 3 is clearly an overestimate, because it does not take into account amplitude fluctuations of the order parameter.

We can get a much clearer picture of the KT transition by searching for vortex and antivortex excitations in the film. Such a picture was first extracted from MC simulations by Tobochnik and Chester (TC),[16] using a nearest-neighbor XY model on a square lattice. Here we can carry their procedure further, since the positions of the vortices and antivortices are described by *continuous* coordinates.

On a discrete lattice, the TC procedure defines the vorticity number q_α of a given plaquette α as

$$q_\alpha = \frac{1}{2\pi} \sum_{\text{bonds}} \Delta\theta , \tag{27}$$

where the sum runs over the bonds enclosing the αth plaquette and $\Delta\theta$ is the phase difference between sites connected by the bond defined so that $-\pi \le \Delta\theta < \pi$. q_α assumes values $+1$ or -1 is there is a positive or a negative vortex inside the plaquette and 0 if there is none.

Figure 2 shows snapshots of the vorticity numbers in model III at several temperatures. Just as found by TC for the nearest-neighbor XY model, there are very few vortices or antivortices for $\mathcal{T} \ll \mathcal{T}_c$, while the number of pairs increases very rapidly as $\mathcal{T} \to \mathcal{T}_c$. The insets of Figs. 2(a) and 2(b) show contour plots of $|\psi(\mathbf{r})|^2$ at the MC times corresponding to these vortex configurations. Here we can clearly identify the vortex and antivortex *cores*. They show up as zeroes of $|\psi(\mathbf{r})|^2$, and may be located anywhere in the plaquettes. (There appears to be no preferred position within the unit cell, because of the evident absence of pinning in this model.) In every plaquette containing a vortex or an antivortex, we find one such zero. Such a zero is required in a vortex-containing plaquette, to keep the current density finite inside the vortex cores. In addition, we sometimes find nonzero minima of $|\psi(\mathbf{r})|^2$ which are associated only with amplitude fluctuations and do not correspond to vortices.

We have also calculated the two-point correlation function

$$\Gamma^{(2)}(\mathbf{r}_0) = \langle \overline{\psi(\mathbf{r})\psi^*(\mathbf{r}+\mathbf{r}_0)} \rangle \tag{28}$$

for model III at several different temperatures. Computationally it is easiest (although not necessary) to evaluate $\Gamma^{(2)}(\mathbf{r}_0)$ at the lattice sites $\mathbf{r}_0 = \mathbf{R}$, since at those sites $\psi(\mathbf{R}) = \psi_0 c_{\mathbf{R}}$. In Fig. 3 we show the arithmetic average

$$\Gamma^{(2)}(r) \equiv \tfrac{1}{2}[\Gamma^{(2)}(r,0) + \Gamma^{(2)}(0,r)] ,$$

obtained by averaging the MC results only over the last 2000 passes. The mean-square order parameter $\langle |\psi|^2 \rangle \equiv \Gamma^{(2)}(0)$ noticeably decreases with temperature, as expected. According to the KT theory, the order-parameter correlation function is expected to die off algebraically at temperatures below $\mathcal{T}_c$ but exponentially above $\mathcal{T}_c$. We have not attempted to fit this prediction to our data, because unambiguous proof of the scaling

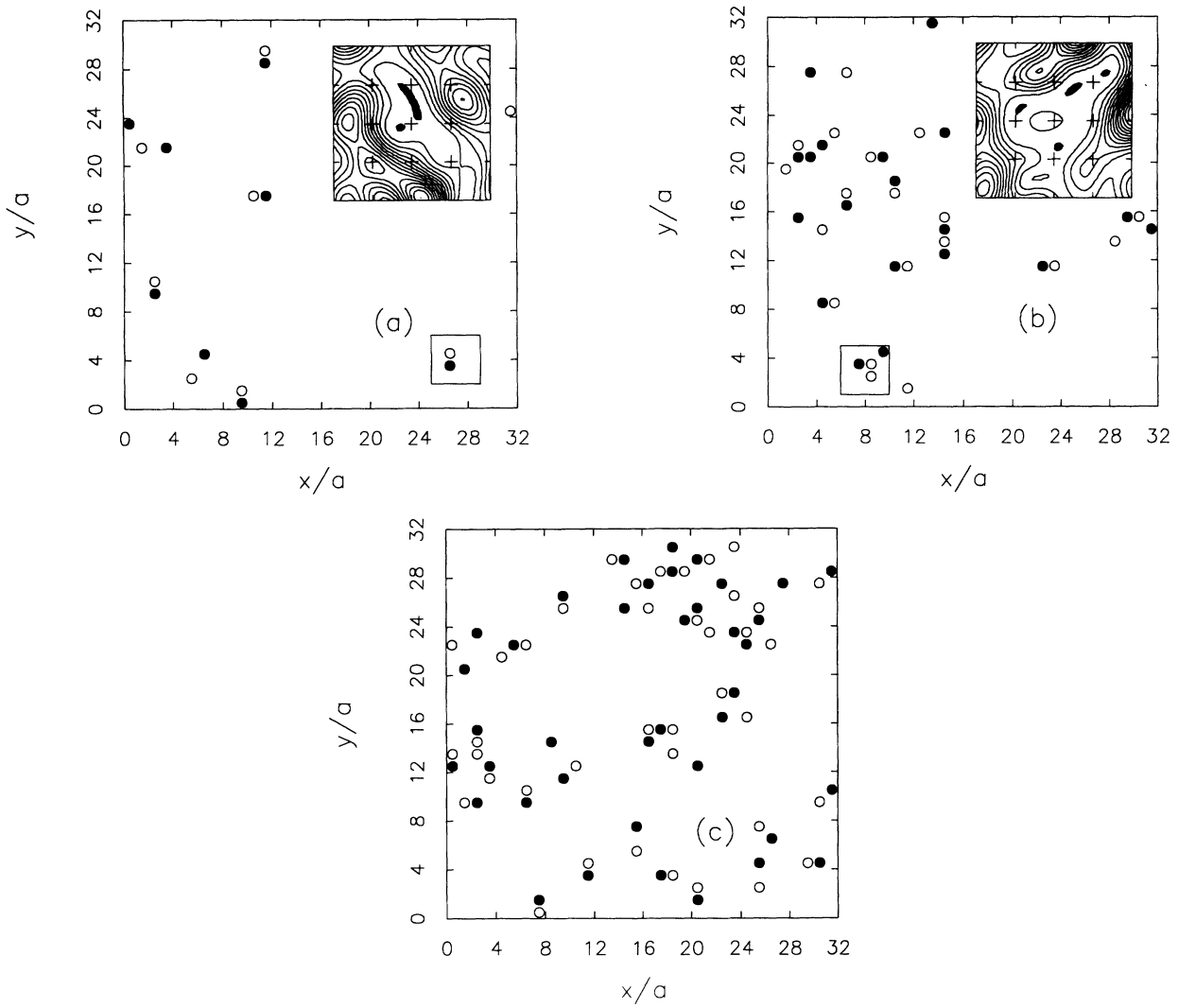

FIG. 2. Snapshots of vortex configurations in model III at temperatures (a) $\mathcal{T}=0.30$, (b) 0.36, and (c) 0.40. The vorticity is defined relative to plaquettes of the square Bravais lattice, and is calculated by the method of Tobochnik and Chester (Ref. 16). Plaquettes containing positive and negative vortices are indicated by ● and ○ symbols; empty plaquettes contain no vortices. The insets are magnified views of framed areas. The contours are loci of constant $|\psi(\mathbf{r})|^2$. The darkened areas are vortex or antivortex cores. Note that both vortices and antivortices correspond to zeroes of the order parameter, and that these zeroes are generally not located at the plaquette centers.

behavior would require larger system sizes than were available to us.

IV. DISCUSSION

It may appear that our results depend on a fictitious lattice constant a, which we have chosen to equal the mean-field correlation length $\xi(T)$. We believe that such a cutoff is actually intrinsic in the Ginzburg-Landau free energy itself. The Ginzburg-Landau model is intended to describe only fluctuations of wavelength larger than

$$\xi(T)=\hbar^2/[2m|\alpha(T)|]^{1/2} .$$

Therefore, it is not appropriate, within this model, to include shorter-wavelength fluctuations in our calculations. By choosing a fictitious lattice constant a of order $\xi(T)$, and keeping only the lowest band of fluctuations, we correctly include only fluctuations of wavelength longer than this expected cutoff. It is true that there is still some degree of arbitrariness in the cutoff, in the sense that we could have chosen $a=K\xi(T)$, with $K\approx 1$ but $K\neq 1$. Each such choice corresponds to a slightly different model, and would lead to slightly different results, as discussed below. The arbitrariness in this model is apparently intrinsic to the choice of a Ginzburg-Landau functional, which does not uniquely specify the short-wavelength cutoff below which fluctuations are to be excluded.[24] A choice $K \gg 1$ would also be possible in principle, though inconvenient, since it would necessitate inclusion of higher Bloch bands in order that all fluctuating modes with wavelength greater than $\xi(T)$ be correctly included. The other extreme choice, $K \ll 1$, would be equally inconvenient, since then most of the first Brillouin zone would involve fluctuations of wavelength

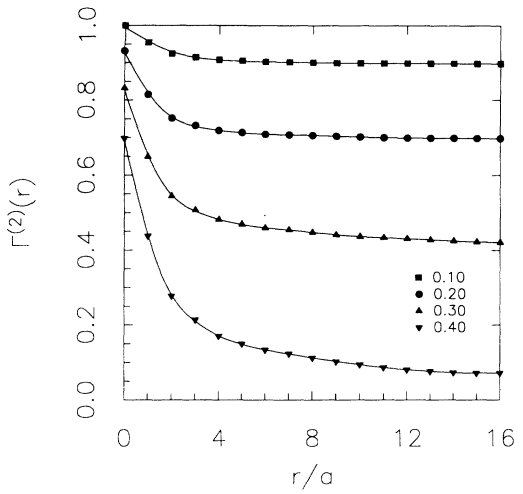

FIG. 3. Correlation function $\Gamma^{(2)}(r)$ plotted as a function of r, in units of ψ_0^2, for model III at several temperatures $\mathcal{T}$ as marked. Note the decrease of $\Gamma^{(2)}(0)$ with increasing $\mathcal{T}$.

much less than $\xi(T)$, which would have to be excluded arbitrarily.

It is of interest to compare our results with those of the Coulomb-gas scaling theory of Minnhagen.[15] This theory predicts that the Coulomb-gas transition temperature $T_c^{CG} \leq \frac{1}{4}$, which translates to $\mathcal{T}_c \leq \pi/4$ in our notation. This is exactly the value denoted by the arrow in Fig. 1. The equality $T_c^{CG} = \frac{1}{4}$ is predicted to hold in the limit of infinite core energy E_c, i.e., if the vortex fugacity

$$z \equiv \exp(-E_c/k_B T) = 0 \ .$$

Clearly, in our model the vortex core has a finite energy, so we should find $\mathcal{T}_c < \pi/4$, which is indeed consistent with our numerical data.

The scaling theory also makes predictions about the universality of the jump in $\gamma(T_c)/k_B T_c$.[22] Namely, the jump is predicted to have its universal value of $2/\pi$ as long as $T_c^{CG} \geq T^*$, where $T^* \approx 0.144$, corresponding to $\mathcal{T}^* \approx 0.45$. In our model III, $\mathcal{T}_c \approx 0.36$. For this value, Ref. 22 predicts a nonuniversal jump of about $3/\pi$, which is indeed consistent with the jump seen in Fig. 1.

It appears that in real *low-T_c* superconducting films, the transition occurs at $T_c \approx 0.476$,[23] where the jump should be universal. This value is somewhat larger than that obtained here. Our model III has several assumptions, however, which could account for this discrepancy. Most notably, the assumption $\mathbf{A}=0$ may not be satisfactory for materials with small κ, as is the case with conventional, low-T_c superconductors with $\kappa \sim 1$. Another is the diagonal approximation to the quartic term and a third is our choice of the dimensionless constant K. The choice $a = K\xi(T)$, where K is a dimensionless constant of order unity, would also guarantee scaling, as well as correctly incorporating only those fluctuations which are described by the original Ginzburg-Landau model, as noted above. But a different choice of K, which is still of order unity, or a more accurate treatment of the quartic term, might raise the $\mathcal{T}_c$ of model III into the universal regime.[24] (A choice $K > 1$ will, in fact, raise $\mathcal{T}_c$, for it suppresses amplitude fluctuations.)

A feature of our model is that it exhibits frustration even in zero magnetic field. This is a characteristic of previous models of superconducting arrays in *finite* fields, which may also exhibit nonuniversal jumps in $\gamma(T_c)/(k_B T_c)$.[20,25] These latter systems, however, usually have, in addition to the continuous rotational symmetry of the XY variable, a discrete Ising-like symmetry.[26] Our model has no obvious symmetry of this kind. It might appear that the frustration is really an artifact of our model, appearing only because of the Wannier basis of oscillating functions. But such oscillating functions are actually required to produce an orthonormal basis in which the uniform ground state can be expanded. Thus, the frustration in our model is evidently *not* an artifact and will be present even if we chose a different—for example, triangular—empty lattice to generate our basis functions, although it may not be strong enough to produce a nonuniversal phase transition.

The present model can readily be extended to 3D layered superconductors. In this case, $T_{c0}(z)$ may be taken as a periodic function of z, the coordinate perpendicular to the layers, with a period d. The order parameter can be expanded in 3D Wannier functions as

$$\psi(\mathbf{r}) = \sum_{\mathbf{R},m} C_{\mathbf{R},m} u_{0\mathbf{R}}(x,y) \phi_m(z) \ ,$$

where $\mathbf{R} \equiv (x,y)$, $\mathbf{r} \equiv (x,y,z)$, m is the layer index, and $\phi_m(z)$ denotes a Wannier function in the z direction, *orthonormalized* according to the relation

$$\int dz \, \phi_m(z) \phi^*_{m'}(z) = \delta_{m,m'} \ .$$

In the tight-binding approximation, only the nearest-neighbor layers interact. As in Ref. 17, the free-energy functional can be expanded in these basis functions, with the result $F = F^{(2)} + F^{(4)}$, where

$$F^{(2)} = a^2 \sum_{\mathbf{R},m} [\alpha(T) + 2t] |C_{\mathbf{R},m}|^2 + \frac{\hbar^2}{2m^*} \sum_{\substack{\mathbf{R},\mathbf{R}' \\ m}} C_{\mathbf{R},m} C^*_{\mathbf{R}',m} U_{\mathbf{R},\mathbf{R}'} - 2ta^2 \sum_{\mathbf{R},m} \Re\{C_{\mathbf{R},m} C^*_{\mathbf{R},m+1}\} \tag{29}$$

and

$$F^{(4)} = \frac{\beta}{2} a^2 w_{0000} \sum_{\substack{\mathbf{R},\mathbf{R}',\mathbf{R}'',\mathbf{R}''' \\ m}} C_{\mathbf{R},m} C_{\mathbf{R}',m} C^*_{\mathbf{R}'',m} C^*_{\mathbf{R}''',m} \times M_{\mathbf{R},\mathbf{R}',\mathbf{R}'',\mathbf{R}'''} \ . \tag{30}$$

Here, $t = \hbar^2/(2m_\parallel^* d^2)$ is the tight-binding matrix element,

$$w_{0000} = \int |\phi_m(z)|^4 dz \ ,$$

and $m_\parallel^*$ is the effective mass along the z axis. Since the anisotropy ratio $m_\parallel^*/m^*$ can be measured, all the coefficients in F can be expressed in terms of a few observable parameters.[17]

The functional form of $\phi_m(z)$ (which determines the value of w_{0000}) depends on the form of $T_{c0}(z)$. This form may be difficult to determine in high-T_c layered systems such as YBCO or BSCCO, but can be written down unambiguously in an artificially layered heterostructure such as MoGe/Ge. In this case, $T_{c0}(z)$ will be a piecewise constant function alternating between the bulk mean-field transition temperatures of the two constituents. Note that the Hamiltonian (29) and (30) omits the magnetic-field-mediated electromagnetic interaction between the superconducting layers. This interaction may be significant in extremely anisotropic materials such as BSCCO,[27] where the Josephson coupling between the layers is small.

It would certainly be of interest to evaluate this model for some naturally or artificially layered superconductors. A simplified version of this model, namely, the anisotropic 3D XY Hamiltonian, has been reported to exhibit a second-order phase transition[28] with a dramatic crossover from 3D to 2D behavior above T_c,[29] corresponding to effective decoupling of pancake vortices in individual superconducting planes. The effects of amplitude fluctuations on this behavior would certainly be worthy of investigation.

To conclude, we have presented an order-parameter expansion for treating phase transitions in 2D superconductors, and have calculated the critical temperature of several approximate versions of this model by Monte Carlo simulation. The most realistic version of this model satisfies the Coulomb-gas scaling relation proposed by Minnhagen,[15] while simultaneously giving a realistic picture of the *spatial* variation of the order parameter $\psi(\mathbf{r})$ at finite temperatures. In particular, $\psi(\mathbf{r})$ exhibits zeroes at the positions of the thermally excited vortices and antivortices. The model exhibits frustration even in zero magnetic field. This may possibly be sufficient, when amplitude fluctuations are included, to produce a nonuniversal jump in the superfluid density at T_c, although approximations in the calculation leave this question open. Finally, the model can be extended straightforwardly to layered superconductors, where a number of applications to high-T_c materials are possible.

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