Order of the metal-to-superconductor transition

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We present results from large-scale Monte Carlo simulations on the full Ginzburg-Landau (GL) model, including fluctuations in the amplitude and the phase of the matter field, as well as fluctuations of the non-compact gauge field of the theory. From this we obtain a precise critical value of the GL parameter $\kappa_{\rm tri}$ separating a first-order metal-to-superconductor transition from a second-order one, $\kappa_{\rm tri}=(0.76\pm0.04)/\sqrt{2}$. This agrees surprisingly well with earlier analytical results based on a disorder theory of the superconductor to metal transition, where the value $\kappa_{\rm tri}=0.798/\sqrt{2}$ was obtained. To achieve this, we have done careful infinite volume and continuum limit extrapolations. In addition we offer an interpretation of $\kappa_{\rm tri}$, namely, that it is also the value separating type-I and type-II behavior.

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I. INTRODUCTION

The character of the metal-to-superconductor transition is an important and long-standing problem in condensed matter physics. The critical properties of a superconductor may be investigated at the phenomenological level by the Ginzburg-Landau (GL) model of a complex scalar matter field ϕ coupled to a fluctuating mass-less gauge field **A**. The GL model in d dimensions is defined by the functional integral

$$Z=\int \mathcal{D}A_i\mathcal{D}\phi\,\exp[-S(A_i,\phi)],$$

$$S=\int d^dx\left[\frac{1}{4}F_{ij}^2+|D_i\phi|^2+m^2|\phi|^2+\lambda|\phi|^4\right], \qquad (1)$$

where $F_{ij}=\partial_iA_j-\partial_jA_i$, $D_i=\partial_i+iqA_i$, q is the charge coupling the condensate matter field to the fluctuating gauge-field, λ is a self-coupling, and m^2 is a mass parameter which changes sign at the mean-field critical temperature. This model is also used to describe a great number of other phenomena in nature, including such widely separated phenomena as the Higgs mechanism in particle physics,[1] phase transitions in liquid crystals,[2,3] crystal melting,[4] and the quantum Hall effect,[5,6] and it is also used as an effective field theory describing phase transitions in the early Universe.[7]

The GL model may conveniently be formulated in terms of two dimensionless parameters $y=m^2/q^4$ and $x=\lambda/q^2$ when all dimensionful quantities are expressed in powers of the scale q^2. Here, y is temperature like and drives the system through a phase transition, and $x=\kappa^2$ is the well-known GL parameter. These parameters are related to the standard dimensionful textbook[8] coefficients α,β of the GL model by

$$y=\frac{m^*c^2}{128\pi^2\alpha_s^2k_{\rm B}^2T^2}\alpha, \quad x=\frac{1}{8\pi\alpha_s\hbar c}\left(\frac{m^*c}{\hbar}\right)^2\beta=\kappa^2, \qquad (2)$$

where α_s is the fine structure constant[9] and m^* is an effective mass parameter.

At the mean-field level Eq. (1) reduces to the well-known GL equations and the model exhibits a second-order phase transition when the temperature (or y) is varied through some critical value. In a seminal paper by Halperin, Lubensky, and Ma[10] it was shown that by ignoring spatial fluctuations in ϕ and then integrating out the **A** field *exactly*, one gets a term $|\phi|^3$ in the effective ϕ action. Treating this action at the mean-field level leads to the prediction of a first-order transition in the charged model for any value of the charge or, equivalently, for any value of the GL parameter. The first-order character of the transition is most strongly pronounced for large values of the charge (small κ), but even then it is very weak. For $\kappa\ll1$ (type I) the neglect of spatial variation in the matter field ϕ is a reasonable approximation, whereas for $\kappa\gtrsim1$ (type II) fluctuations in ϕ must be taken into account. By doing a one-loop renormalization group (RG) calculation using the ε expansion it was shown[10] that no stable infrared fixed point could exist unless the number N of components of the order parameter was artificially extended to $N>N_c=365$, far beyond the physically relevant case of $N=2$. Consequently, the conclusion was that gauge field fluctuations change the order of the phase transition to first order *irrespective* of the value of κ.

These predictions were difficult to test experimentally on superconductors since the predicted jump across the first-order transition is very small in *physical* units, even if the *effective* theory in Eq. (1) has a strong first-order transition. See, e.g., Appendix A in Ref. 11. For conventional superconductors the critical region where mean-field behavior breaks down is extremely narrow; consequently, it is very difficult to distinguish a small finite jump from continuous behavior. However, there exists an isomorphism between the phase transition in superconductors and the smectic-A to nematic transition in liquid crystals.[12] On the latter systems experiments can be carried out in the critical regime,[13] and second-order phase transitions are found. This contradicts the ϵ-expansion argument above and presumably indicates a breakdown of the expansion for this gauge-field theory, since $\varepsilon=4-d=1$.

In Ref. 14 it was shown, using duality arguments and Monte Carlo simulations, that the GL model should have a

second-order transition for large κ. However, what remains true is that deep in the type-I regime, the transition *is* first order. There should therefore be a tricritical point $\kappa=\kappa_{\rm tri}$ where the transition changes order.

A first estimate for $\kappa_{\rm tri}$ was obtained by Kleinert in Refs. 15 and 16 by developing a disorder theory formulation from which he calculated the value

$$\kappa_{\rm tri}=\frac{3\sqrt{3}}{2\pi}\sqrt{1-\frac{4}{9}\left(\frac{\pi}{3}\right)^4}\approx\frac{0.798}{\sqrt{2}}$$

analytically.[17] Subsequently[18] this picture of a tricritical point separating first- and second-order transitions was given further support by Monte Carlo simulations, and moreover an attempt was even made to determine $\kappa_{\rm tri}$, giving $\kappa_{\rm tri}\simeq 0.4/\sqrt{2}$. However, the problem turns out to be extremely demanding even by present day supercomputing standards, and not too much emphasis can be put on the *precise numerical value* obtained in this early attempt. To our knowledge, this is the most recent attempt to find a precise value for $\kappa_{\rm tri}$ numerically, although large-scale simulations have been performed much more recently for $\kappa^2=0.0463$ and $\kappa^2=2$, giving first-order and continuous transitions, respectively.[11,19]

The one-loop ε-expansion result of Halperin *et al.*[10] has subsequently been improved to two-loop order.[20] Eventually, an infrared stable fixed point was found even for the physical case $N=2$ by combining two-loop perturbative results with Padé-Borel resummation techniques.[21] From this latter work one can also get an estimate of the critical κ from $\kappa^*=\sqrt{u^*/6f^*}\approx 0.62/\sqrt{2}$. Since Padé-Borel techniques are rather uncontrolled, only simulations can tell if such a resummation is allowed here.

From the above we can conclude that a tricritical κ, separating first- and second-order transitions, *exist* however a *precise value* remains to be determined.

We would also like to mention the distinction between type-I and type-II superconductors, which is related to the response to an external magnetic field. When an external field is increased beyond a critical field H_c it enters a type-I superconductor, and superconductivity is destroyed. For type-II superconductors the magnetic field enters as *a flux line lattice* when $H>H_{c1}$, and superconductivity is still present in this mixed state. At the mean-field level type-I and type-II superconductors are differentiated by $\kappa=1/\sqrt{2}$. However, there is *a priori* no reason to assume that this numerical value is robust against fluctuation effects, and we will argue that the critical κ separating first- and second-order phase transitions coincides with the κ separating type-I and type-II superconductors at y_c.

II. ORDER OF THE TRANSITION

The model in Eq. (1) has a phase transition for $y=y_c$. For $y<y_c$ the system is in its superconducting (broken) phase while for $y>y_c$ it is in the normal (symmetric) phase. Note that here, broken and symmetric do not refer to a breakdown of the local gauge symmetry present in Eq. (1). Elitzur's theorem[22] states that a local symmetry can never be spontaneously broken and therefore no local order parameter (in general any non-gauge-invariant order parameter) can exist. On the other hand, one can explicitly break the gauge symmetry by a gauge fixing, thereby facilitating a meaningful definition of a local order parameter. This should nonetheless be chosen in a formally gauge-invariant manner to get gauge-independent results. In our simulations, we have chosen not to fix the gauge.[23] In this case a phase transition must be found either by using *nonlocal*[19,24] order parameters or by looking for non analytic behavior in local quantities,[11] as we have done. E.g., the quantity $\langle|\psi|^2\rangle$ will have a jump at a first-order transition, but it will not disappear in the symmetric phase as a proper order parameter should. At a second-order transition there will be no jump, but the susceptibility $\chi_{|\psi|^2}$ will still have a peak.

In principle, we could therefore decide the order by looking for a jump in some local quantity as $\langle|\psi|^2\rangle$, but in finite systems the discontinuity will be rounded. In our case this is particularly problematic since the first-order transitions are very weak, giving small jumps, even in infinite systems. At a first-order transition ordered and disordered phases coexist and have the same free energy. In a finite system there will therefore be oscillations between the different phases. Because of the surface energy between the two pure states, the probability of finding the system in an intermediate mixed state is lower than for either of the pure states, and histograms of an arbitrary observable will show a pronounced double-peak structure. This is in contrast to a second-order transition where the diverging correlation length forbids coexistence since the whole system is correlated. The histograms then have a single peak. Typical histograms are shown in Fig. 2, below.

Thus, when these histograms have a double-peak structure which becomes more pronounced when the system size increases, the transition is first order, otherwise not.[25]

More precisely, we have the following scaling for the difference in free energy between the mixed and pure phases for sufficiently large $L>L_{\rm scaling}$:

$$\Delta F(L)=\ln P(X,L)_{\rm max}-\ln P(X,L)_{\rm min}\sim L^{d-1}, \qquad (3)$$

where $P(X,L)$ is the probability for a given observable X in a system of size L^d, and L^{d-1} is the cross-sectional area between the ordered and disordered phases. Near the tricritical value of κ such scaling is difficult to achieve since we are interested in the limit of vanishingly weak first-order transitions. Consequently, a very large L is required in order to observe proper scaling. Only for quite strong first-order transitions have we been able to observe proper scaling as predicted by Eq. (3); however, we have generally taken a monotonous increase in $\Delta F(L)$ with system size as a signature of a first-order phase transition. For the weakest first-order transitions $\Delta F(L)$ will typically decrease for small L and then start to increase. It is therefore important to observe monotonic behavior through several system sizes before a conclusion can be drawn from the histograms.[26]

III. PHASE DIAGRAM

We are searching for the point in the (x,y) plane where a first-order and a second-order line meet; i.e., according to the rather loose definition[27] of Lawrie and Sarbach[28] we are looking for a *tricritical point*. At a tricritical point *two* coupling constants must be fine-tuned to nontrivial values, and consequently a tricritical theory can be described with the mean-field free energy

$$f \approx |\nabla \psi|^2 + c_1(y - y_{\rm tri})|\psi|^2 + c_2(x - x_{\rm tri})|\psi|^4 + c_3|\psi|^6. \tag{4}$$

Right at the tricritical point the coefficients in front of both $|\psi|^2$ and $|\psi|^4$ vanish *simultaneously*. The upper critical dimension for this model is $d^*=3$ and mean-field theory should be valid (up to logarithmic corrections). When approaching the tricritical point from the first-order side, mean-field theory predicts that the jump $\Delta|\psi|^2$ will vanish as

$$\Delta|\psi|^2 \sim (x_{\rm tri} - x). \tag{5}$$

We will make use of the above scaling in Sec. VI to estimate $x_{\rm tri}$. For further information about tricritical points, we refer to an extensive review by Lawrie and Sarbach.[28]

In Fig. 1 we have *assumed* that the tricritical point separating first- and second-order phase transitions coincides with the point separating type-I and type-II superconductivity. In principle the line of second-order transitions could extend into the type-I region, with an intermediate state of type-I superconductivity with a second-order phase transition to the normal state. This would be the case if the mean-field value $\kappa_{\rm I/II}=1/\sqrt{2}$ were *not* renormalized by fluctuations. We have not focused on the aspect of type-I and type-II superconductivity in our simulations; we will, however, argue that the overall structure of the phase diagram shown in Fig. 1 is correct in the vicinity of the tricritical point.

The microscopic difference between type-I and -II superconductors lies in the sign of the effective vortex-vortex interaction. In $d=3$ there exists a *dual* formulation of the GL model which is given by a complex scalar matter field ϕ coupled minimally to a massive gauge field. This gauge field can thus safely be integrated out to yield an effective *local* $|\phi|^4$ theory, where the coefficient of the $|\phi|^4$ term gives the effective vortex-vortex interaction. A positive such term signals vortex repulsion, i.e., type-II behavior, while a negative term signals type-I behavior. *This vortex-vortex interaction term is proportional to* $\kappa - \kappa_{\rm tri}$ where $\kappa_{\rm tri}$ is indeed to be identified with our tricritical value of κ.[15] Using the dual formulation of the GL theory, it then becomes clear that $\kappa_{\rm tri}$ is at the same time the value that separates first- and second-order behavior, *and* the value that separates attractive from repulsive effective vortex-vortex interactions, i.e., type-I from type-II behavior.

An independent argument for why the transition between the normal state and type-I superconductivity *must be first order* is based on the geometrical properties of a vortex tangle: In a recent paper[29] we have calculated the fractal dimension of vortex loops and found the scaling relation $\beta = \nu(d - D_{\rm H})/2$, where β is the order parameter exponent, ν is the correlation length exponent, and $D_{\rm H}$ is the fractal dimension of the loops. If we formally extend this relation to the first-order regime, i.e., let $\beta \to 0^+$, we find that the fractal dimension of the vortex loops $D_{\rm H} \to d$—i.e., the vortices collapse on themselves (filling space completely)—rendering the transition discontinuous. This collapse is what we would expect from vortices interacting attractively (i.e., type I), and by turning the argument above around we conclude that type-I superconductors must have a first-order transition to the normal state.

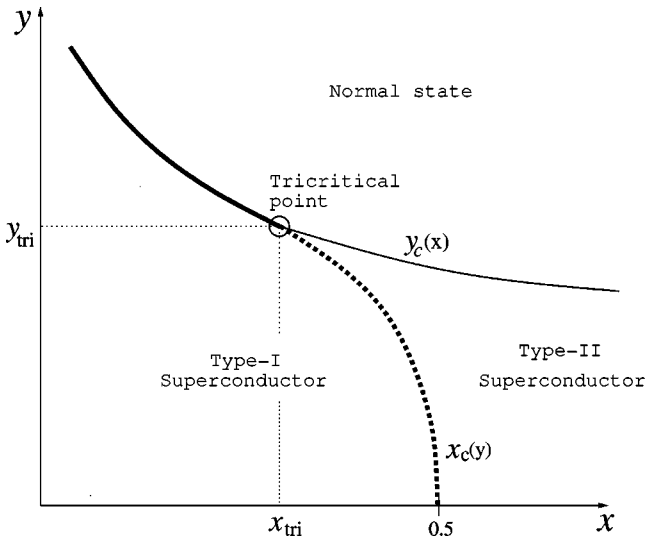

FIG. 1. A conjectured phase diagram in the (x,y) plane *in the vicinity of the tricritical point*. The thick solid line is a line of first-order transitions separating type-I superconductivity and the normal (metallic) state, and the thin solid line is a second-order line separating type-II superconductivity from the normal (metallic) state. The dashed line separates type-I and type-II superconductivity. The dotted horizontal and vertical lines indicate the coordinates of the tricritical point $(x_{\rm tri}, y_{\rm tri}) \simeq (0.30, 0.03)$.

We emphasize that the detailed *shape* of the line $x_c(y)$ remains to be determined. We have presented arguments above that it ends in the tricritical point $(x_{\rm tri}, y_{\rm tri})$. Moreover, deep in the broken regime, mean-field theory should apply. Consequently, we expect that the line $x_c(y)$ converges towards the mean-field value $x_{\rm I/II}=1/2$ in the $y \to -\infty$ limit.

IV. LATTICE MODEL

To perform simulations on the model in Eq. (1) we define it on a numerical lattice of size $N \times N \times N$ with lattice constant a. The *physical* volume is then $V = L^3 = (Na)^3$. By introducing a lattice field given by

$$|\phi_{\rm (cont)}|^2 = \beta_H |\psi_{\rm (latt)}|^2 / 2a, \tag{6}$$

where β_H so far is an arbitrary constant, Eq. (1) takes the form

$$Z = \int \mathcal{D}A_i \mathcal{D}\psi \exp[-S(A_i, \psi)]$$

$$S=\beta_G\sum_{x,i<j}\frac{1}{2}F_{ij}^2-\beta_H\sum_{x,i}\mathrm{Re}[\psi^*(\vec{x})U_i(\vec{x})\psi(\vec{x}+\hat{i})]$$
$$+\frac{\beta_H}{2}\left[6+\frac{y}{\beta_G^2}\right]\sum_{\vec{x}}|\psi|^2+\beta_R\sum_{\vec{x}}|\psi|^4, \quad (7)$$

where we have defined $\alpha_i(\vec{x})=aqA_i(\vec{x})$, $U_i(\vec{x})=e^{i\alpha_i(\vec{x})}$, $\beta_G=1/a_q$, $F_{ij}=\alpha_i(\vec{x})+\alpha_j(\vec{x}+\hat{i})-\alpha_j(\vec{x})-\alpha_j(\vec{x}+\hat{j})$, and $\beta_R=x\beta_H^2/4\beta_G$. Here F_{ij} is essentially a lattice curl of the fluctuating gauge field, and $a_q=aq^2$ is a dimensionless lattice constant. To obtain correct continuum limit results, we will ultimately be interested in the limit $a_q\to 0$. It is furthermore possible to select a value of β_H such that the action can be written in the form

$$S=\beta_G\sum_{x,i<j}\frac{1}{2}F_{ij}^2-\beta_H\sum_{x,i}\mathrm{Re}[\psi^*(\vec{x})U_i(\vec{x})\psi(\vec{x}+\hat{i})]$$
$$+\sum_{\vec{x}}|\psi|^2+\beta_R\sum_{\vec{x}}[|\psi|^2-1]^2. \quad (8)$$

This is achieved provided β_H satisfies the relation $(\beta_H/2)\times[6+y/\beta_G^2]+2\beta_R=1$.

The amplitude and gauge-invariant phase difference $\Delta=\arg[\psi^*(\vec{x})U_i(\vec{x})\psi(\vec{x}+\hat{i})]$ are coupled through the second term in Eq. (8). The ordered state is characterized by $\cos\Delta\lesssim 1$ and $|\psi|$ close to the minimum in the potential energy, whereas in the disordered state $\cos\Delta\approx 0$. In the disordered state the amplitude behavior is determined by x; for small x the coupling to Δ dominates and $|\psi|$ deviates significantly from the minimum in the potential, whereas for large x amplitude fluctuations are suppressed.

Given the fact that the theory in Eq. (1) is a continuum theory, one has to perform an ultraviolet (short-distance) renormalization, and thus $m^2=m^2(q^2)$ has to be interpreted as a renormalized mass parameter at a given scale q^2 within a given renormalization scheme, e.g., the minimal subtraction ($\overline{\mathrm{MS}}$) scheme. Since this continuum theory should represent the $a\to 0$ limit of the lattice theory in Eq. (8), the parameter y must be varied when a is being varied. In our case the leading terms in a can be obtained by requiring that some physical correlator calculated in both lattice and continuum perturbation theory should coincide. Thus we have to make the substitution[30,31]

$$y\to y-\frac{3.1759115(1+2x)}{2\pi}\beta_G$$
$$-\frac{(-4+8x-8x^2)[\ln(6\beta_G)+0.09]-1.1+4.6x}{16\pi^2}$$
$$+\mathcal{O}(1/\beta_G). \quad (9)$$

In addition, the continuum and lattice condensate matter fields are related by

$$\frac{\langle\phi^*\phi\rangle_{\mathrm{cont}}}{q^2}=\frac{\beta_H\beta_G}{2}\langle\psi^*\psi\rangle_{\mathrm{latt}}-\frac{3.175911\beta_G}{4\pi}$$
$$-\frac{\ln(6\beta_G)+0.668}{8\pi^2}+\mathcal{O}(1/\beta_G). \quad (10)$$

In Eq. (10) the first term comes from Eq. (6), while the second and third terms are linear and logarithmic divergences due to renormalization.

Note that the complicated counterterms in Eq. (9) merely affect the *value* of y_c separating the normal from the superconducting state for a given x, not the overall *structure* of the phase diagram. The divergences in Eq. (10) in the continuum limit are constants that cancel when the jump in $\langle\phi^*\phi\rangle$ across a first-order phase transition is calculated.

V. DETAILS OF SIMULATIONS

In order to use Eq. (8) to study the continuum theory of Eq. (1), it is necessary to carefully take two limits separately. First, the infinite-volume limit $L\to\infty$ is taken; thereafter, the continuum limit $a\to 0$. For reliable results one should have $a\ll\xi\ll L$, where ξ is a typical correlation length for the problem. In statistical physics, the continuum limit is usually not considered, either because the models are inherently *lattice models* or the models are studied around a second-order critical point where there exists at least one diverging length scale. Under such circumstances the short length-scale properties, like the lattice constant, are rendered irrelevant when studying universal properties. On the other hand, if one wants to study nonuniversal properties (such as critical coupling constants) or first-order transitions without a diverging length scale, details of the system even on the shortest length scales have to be correctly taken into account in order to give reliable results.

The Monte Carlo simulations are performed on Eq. (8), updating phases, amplitudes[32] and gauge fields. We have used periodic boundary conditions and noncompact gauge fields without any gauge fixing. To reduce autocorrelation times we have added global updating of the amplitude and overrelaxation of the scalar field[33,34] such that one sweep consists of (1) conventional local Metropolis updates for phase, amplitude, and gauge field, (2) global radial update by multiplying the amplitude uniformly with a common factor (acceptance according to Metropolis dynamics), and (3) two to three overrelaxation ''sweeps'' updating both the amplitude and the phase of the scalar field. The acceptance ratio in the Metropolis steps is kept between 60% and 70% as long as possible by adaptively adjusting the maximum allowed changes in the fields. For further details of the technical aspects of the simulations, see Refs. 33 and 34.

We have performed simulations for the parameters in Table I. The simulations have been done in a hierarchical manner: For a given x we have first kept a_q and N fixed, and simulated on typically three to eight y values. These runs have been combined with Ferrenberg-Swendsen[35,36] reweighting techniques, and a (pseudo)critical y has been located by requiring that the reweighted histograms have two equally high[37] peaks. Then the system size has been increased

TABLE I. The lattice sizes N^3 used for each (a_q, x) pair. For each lattice size typically between three and eight y values were used. The symbols are defined by ○ (not simulated), ⋆ (simulated), and ● (simulated and results shown in Fig. 2).

a_q	x	N									
		8	12	16	20	24	32	40	48	64	96
5.0[a]	0.10	⋆	○	○	○	○	○	○	○	○	○
	0.15	⋆	⋆	⋆	⋆	⋆	⋆	○	○	○	○
	0.16	⋆	⋆	●	●	●	●	○	○	○	○
	0.17, 0.18, 0.19	⋆	⋆	●	○	●	●	●	○	○	○
2.0	0.10	⋆	⋆	○	○	○	○	○	○	○	○
	0.15	⋆	⋆	⋆	○	○	○	○	○	○	○
	0.20	⋆	⋆	⋆	○	⋆	⋆	⋆	○	○	○
	0.22	○	○	●	○	●	●	●	○	○	○
	0.23, 0.24, 0.25	○	○	●	○	●	●	●	○	●	○
1.0	0.08	⋆	⋆	⋆	○	○	○	○	○	○	○
	0.10	⋆	⋆	⋆	⋆	○	○	○	○	○	○
	0.12, 0.13, 0.14	⋆	⋆	⋆	○	⋆	⋆	○	○	○	○
	0.15, 0.16, 0.17	○	⋆	⋆	⋆	⋆	⋆	⋆	○	○	○
	0.18, 0.20	⋆	⋆	⋆	○	⋆	⋆	⋆	⋆	○	○
	0.22	⋆	⋆	⋆	○	⋆	⋆	⋆	⋆	⋆	○
	0.24, 0.25, 0.26, 0.27	⋆	⋆	●	○	●	●	●	●	●	○
	0.30	⋆	⋆	⋆	○	⋆	⋆	⋆	⋆	○	○
	0.50	○	○	⋆	⋆	⋆	⋆	⋆	○	○	○
0.5	0.16	○	○	○	○	●	●	●	●	○	○
	0.20, 0.24	○	○	○	○	●	●	●	●	●	○
	0.26, 0.28	○	○	○	○	●	●	●	●	●	●
	0.30	○	○	○	○	●	●	●	●	●	○

[a]In Ref. 18 the lattice spacing corresponds to $a_q = 5.0$. The system sizes used were 9^3 and 15^3.

to access the *infinite-volume limit*, and finally we have varied a_q to determine the *continuum limit*. At the transition the number of sweeps was chosen so that the system oscillated back and forth between the ordered and disordered states about 10 times. Depending on system size and x value (i.e., the *strength* of the first-order transition) this resulted in about 10^5–10^6 sweeps. All computations were performed on an SGI Origin 3800 at the Norwegian High Performance Computing Center, using up to 32 nodes in parallel for the largest systems. A total of about 5×10^4 CPU hours were used, corresponding to $\simeq 1.5\times10^{17}$ floating point operations.

VI. RESULTS

To find $x_{\rm tri} = \kappa^2_{\rm tri}$ our strategy has been to start at $x \ll x_{\rm tri}$ where the transition is clearly first order, and then slowly increase x into the problematic tricritical area where $x \lesssim x_{\rm tri}$. During the simulations we have sampled the lattice amplitude

$$\overline{|\psi|^2} = \frac{1}{N^3}\sum_{\vec{x}} |\psi(\vec{x})|^2 \tag{11}$$

and histograms of this quantity constitute the raw data for most of the subsequent analysis.[38] The connection between continuum and lattice condensates is given by Eq. (10).

Histograms reweighted to the critical y value are shown in Fig. 2. We have used two different methods to find $x_{\rm tri}(a_q)$ from the histograms, and finally at the end of this section we have extrapolated these values to $a_q = 0$ to find the continuum limit.

A. Extrapolation of $\Delta\overline{|\psi|^2}$ to zero

The distance between the peaks of a histogram gives $\Delta\overline{|\psi|^2}(N)$, and by computing this for several different system sizes one can compute the infinite-volume limit $\lim_{N\to\infty}\Delta\overline{|\psi|^2}$ of the discontinuity at the transition. Then one can (in principle) extrapolate to larger x and find the value $x_{\rm tri}$ where the discontinuity disappears. Results for $\lim_{N\to\infty}\Delta\overline{|\psi|^2}$ as a function of x are shown in Fig. 3.

For small x the curves in Fig. 3 show a distinct positive curvature, but when approaching $x_{\rm tri}$ we find that $\Delta\overline{|\psi|^2}$ vanishes as $\propto(x_{\rm tri}-x)$, in accordance with mean-field theory, Eq. (5). Also in the original attempt to locate $x_{\rm tri}$ with Monte Carlo simulations[18] this extrapolation was done; however,

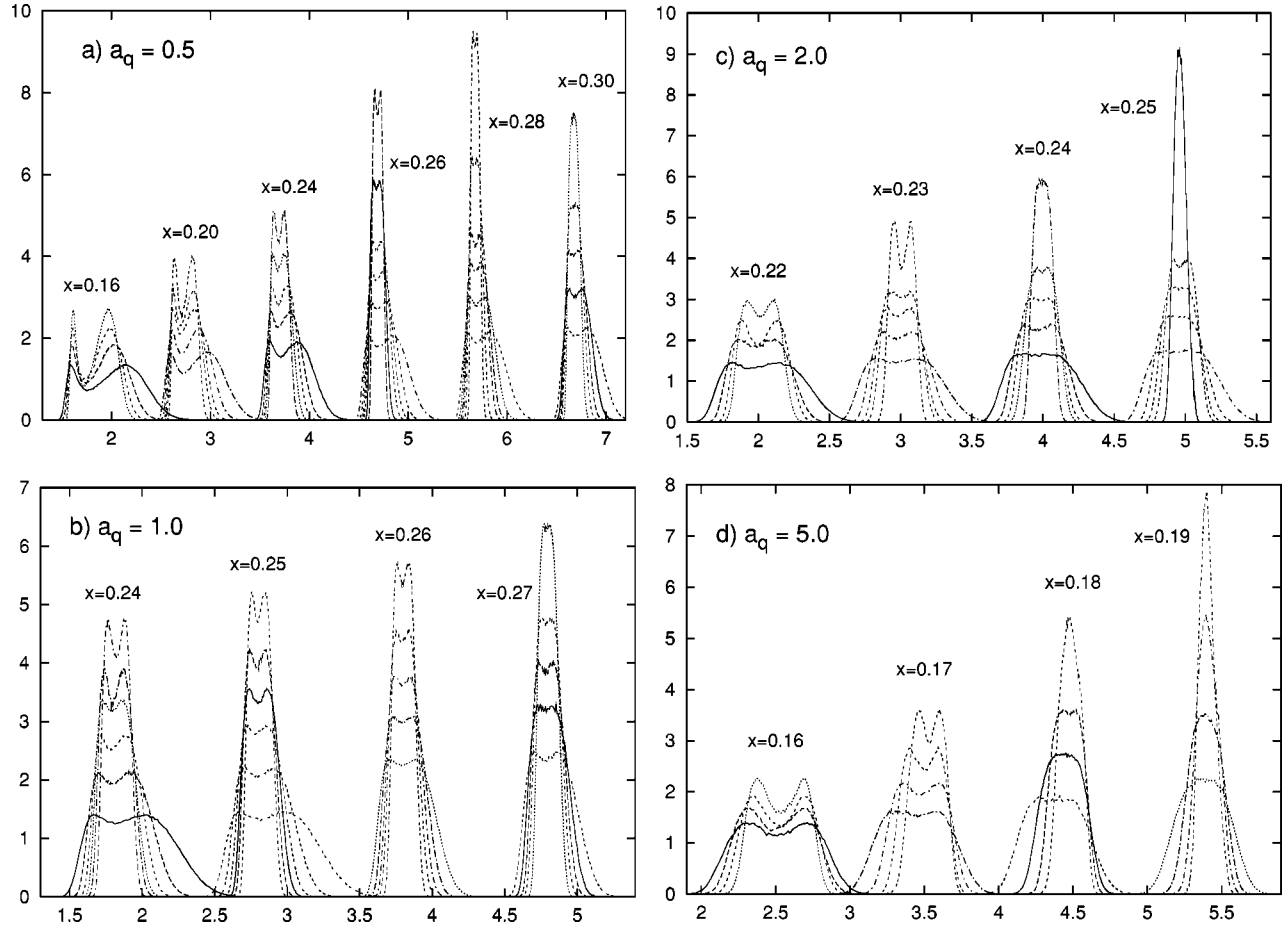

FIG. 2. Normalized histograms $P(\overline{|\psi|^2})$ as a function of $\overline{|\psi|^2}$ for (a) $a_q=0.5$, (b) $a_q=1.0$, (c) $a_q=2.0$, and (d) $a_q=5.0$. For each lattice spacing the histograms for the smallest x are correctly placed horizontally. For larger x they are offset horizontally in steps of 1 for clarity. For system sizes see Table I.

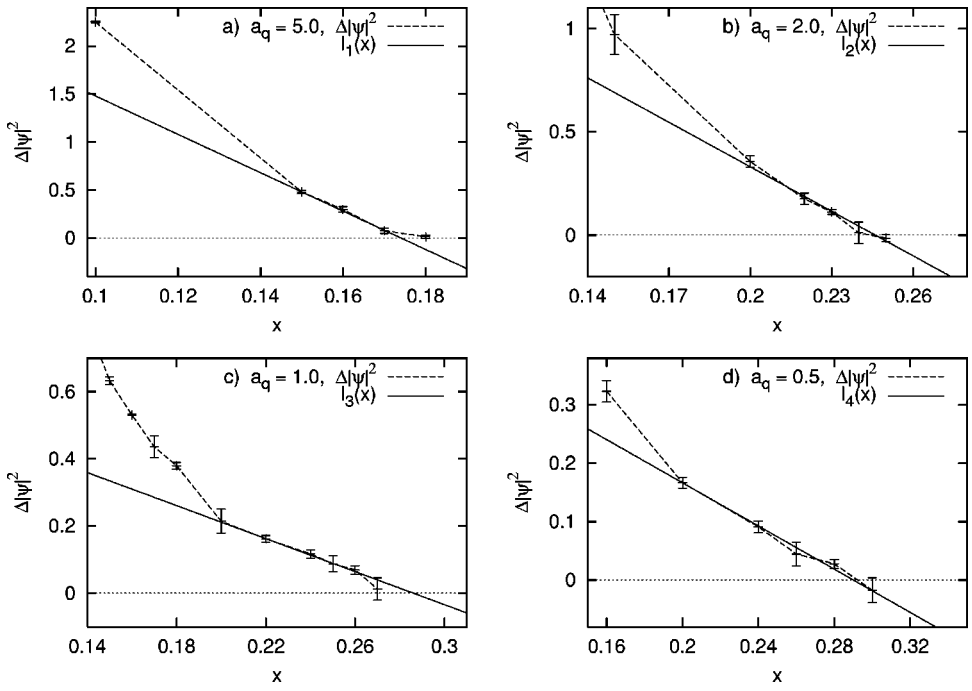

FIG. 3. $\lim_{N\to\infty}\Delta\overline{|\psi|^2}$ as a function of $x=\kappa^2$ for the lattice constants (a) $a_q=5.0$, (b) $a_q=2.0$, (c) $a_q=1.0$, and (d) $a_q=0.5$. The line $l_i(x)$, $i=1,\ldots,4$, is a fit to Eq. (5) where x_c is given in Table II.

TABLE II. $x_{\rm tri}$ found from extrapolation of $\lim_{N\to\infty}\Delta\overline{|\psi|^2}$ to zero and finite-size scaling of $\Delta F(N)$.

a_q	$x_{\rm tri}$ (from $\Delta\overline{\lvert\psi\rvert^2}$)	$x_{\rm tri}$ (from $\Delta F(N)$)
5.0	0.174 ± 0.002	0.175 ± 0.005
2.0	0.246 ± 0.002	0.235 ± 0.005
1.0	0.286 ± 0.010	0.260 ± 0.010
0.5	0.294 ± 0.005	0.280 ± 0.020

the extrapolation was done starting from quite small x values, and the resulting $x_{\rm tri}$ was much smaller than the one we calculate.

The extrapolated results for $x_{\rm tri}$ are shown in Table II. The values found should provide a reasonable upper limit for $x_{\rm tri}(a_q)$.

B. Finite-size scaling of $\Delta F(N)$

It is also possible to study the *height* of the peaks in the histograms $[P(\overline{|\psi|^2})_{\rm max}]$ relative to the minimum between them $[P(\overline{|\psi|^2})_{\rm min}]$. This constitutes the best method of determining whether a transition is first order or not, but one cannot extrapolate to find $x_{\rm tri}$. In Fig. 4 we show some typical results for $\Delta F(N)=\ln P_{\rm max}-\ln P_{\rm min}$ as a function of system size N for $a_q=0.5$.

For $x=0.16$ we clearly see the scaling $\Delta F(N)\propto N^2$ for $N\gtrsim 40$. This is expected since the histograms in Fig. 2 show a very pronounced double-peak structure. For larger x this becomes less clear. Our estimates of $x_{\rm tri}$ for the different lattice constants are given in Table II. The results are consistently somewhat below those found with the method given in Sec. VI A and give a reasonable lower limit for $x_{\rm tri}$.

C. Other methods

Finite-size scaling of the maximum in susceptibilities of the quantities $\overline{|\psi|^2}$ and $\overline{L}$ gives results that are consistent with the above conclusions:

$$\chi_S=N^d(\langle S^2\rangle-\langle S\rangle^2)\sim N^\sigma,\quad S\in\{\overline{|\psi|^2},\overline{L}\},\qquad(12)$$

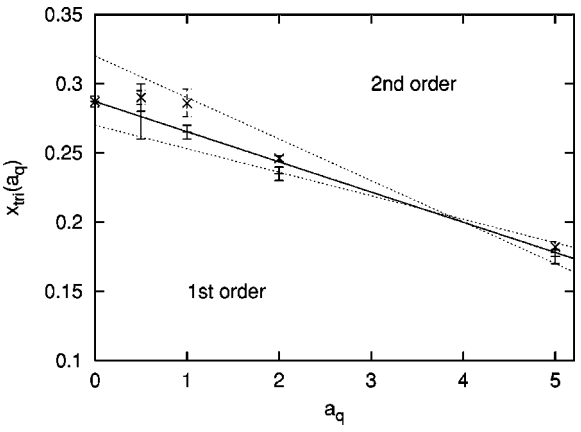

FIG. 5. Plot of $x_{\rm tri}(a_q)$ using the results from extrapolation of $\Delta\overline{|\psi|^2}$ to zero and from finite-size scaling of $\Delta F(N)$ given in Table II. The solid line is a linear fit giving $\lim_{a_q\to 0}x_{\rm tri}(a_q)=0.287\pm0.004$. The dotted lines indicate ''worst case scenarios'' giving $\lim_{a_q\to 0}x_{\rm tri}(a_q)=0.295\pm0.025$.

where $\sigma=d(<d)$ for first- (second-) order transitions. However, these results are more ambiguous than those from the histograms, and we have therefore chosen to work mainly with the histograms.

D. Final result for $\kappa_{\rm tri}$

It is clear that it becomes increasingly difficult to obtain good estimates of $\kappa_{\rm tri}(a_q)$ when the lattice constant is reduced. This is easy to understand since the *physical* volume $(Na_q)^3$ will be drastically reduced for the same lattice size in lattice units. The size of N necessary to access the scaling regime is (approximately) inversely proportional to the lattice constant a_q.

In Fig. 5, we show $x_{\rm tri}(a_q)$ found from extrapolation of $\Delta\overline{|\psi|^2}$ to zero and from finite-size scaling of $\Delta F(N)$ as given in Table II. A linear fit to the data gives $\lim_{a_q\to 0}x_{\rm tri}(a_q)=0.287\pm0.004$ with a confidence level of 25%. This is probably an underestimate of the error, since we have no particular reason to assume a linear behavior. Since the errors in $x_{\rm tri}(a_q)$ increases considerably when we reduce a_q one can-

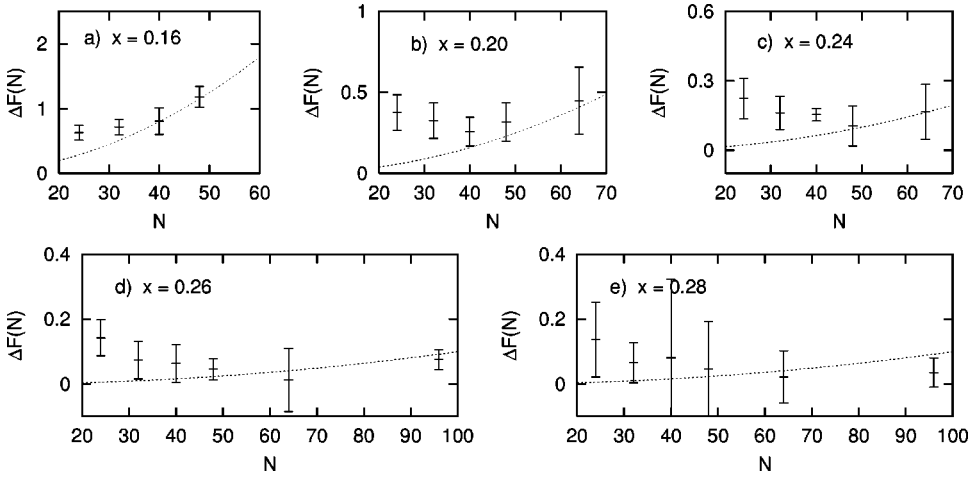

FIG. 4. $\Delta F(N)=\ln P_{\rm max}(N)-\ln P_{\rm min}(N)$ for $a_q=0.5$. The line is $\propto N^2$ which is the scaling in Eq. (3) (for $d=3$).

not rule out other behaviors, as quadratic. From the ''worst case scenario'' shown by the dotted lines in the figure we get $\lim_{a_q \to 0} x_{\rm tri}(a_q) = 0.295 \pm 0.025$. This in all likelihood gives a more realistic estimate of the error, and we therefore give our final estimate of $\kappa_{\rm tri}$ as $\lim_{a_q \to 0} \kappa_{\rm tri}(a_q) = (0.76 \pm 0.04)/\sqrt{2}$.

VII. CONCLUSION

In summary, we have presented results from large-scale Monte Carlo simulations showing that the critical value of the Ginzburg-Landau parameter that separates first-order from second-order behavior at the superconductor–normal-metal transition point, is $\kappa_{\rm tri} = (0.76 \pm 0.04)/\sqrt{2}$. This is in remarkable agreement with the first estimate of $\kappa_{\rm tri}$ obtained by Kleinert[15] using a mean-field theory on the dual of the Ginzburg-Landau model, but differs almost by a factor of 2 from the subsequent early simulation results of Bartholomew.[18]

The reason for the remarkable agreement with our result and those of Ref. 15, is that for small to intermediate values of κ, the original problem is in the strong-coupling regime and is mapped onto a weak-coupling problem in the dual formulation. The dual model is then expected to yield rather precise results at the mean-field level.[15] The dual description of the Ginzburg-Landau model has recently met with considerable success in predicting the phase structure of extreme type-II superconductors, even in magnetic fields.[39–42] We interpret the good agreement between our results and those of Ref. 15 as further support of the dual description of the Ginzburg-Landau model, now also in the intermediate-κ region.

We have also argued that this $\kappa_{\rm tri}$ coincides with the κ separating type-I and type-II superconductivity. In the superconducting regime for $\kappa \in (\kappa_{\rm tri}, 1/\sqrt{2})$ we thus predict the possibility of going from type-I to type-II superconductivity by increasing the temperature. This could in principle be possible to observe by studying the vortex structure of a superconductor with such intermediate values of κ by small-angle neutron scattering, when lowering the temperature through the line $x_c(y)$. However, more work is needed to elucidate the properties of the line $x_c(y)$ in Fig. 1.

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[27] Indeed, it has been customary to describe as ''tricritical'' any point at which a continuous transition becomes discontinuous, irrespective of the number of phases which coexist along the first-order line or of the number of lines or surfaces of ordinary

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[38] In addition to $\overline{|\psi|^2}$ we have also studied other quantities, in particular

$$\overline{L} = \frac{1}{3N^3} \sum_{\mathbf{x},i} \cos\{\arg[\psi^*(\vec{x}) U_i(\vec{x}) \psi(\vec{x}+\hat{i})]\},$$

which varies between zero in the symmetric state and one in the broken state, quite similar to the more familiar 3D *XY* quantity $\langle \cos(\theta(\mathbf{x}) - \theta(\mathbf{x}+\hat{i})) \rangle$. However, the general picture is that the different observables give essentially the same information, and we have therefore focused mainly on Eq. (11), which has a well-defined continuum limit.

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