The 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 \( \kappa_{\text{tri}} \) separating a first order metal to superconductor transition from a second order one, \( \kappa_{\text{tri}} = (0.76 \pm 0.04)/\sqrt{2} \). This agrees surprisingly well with earlier analytical results based on a disorder theory of the superconductor to metal transition, where the value \( \kappa_{\text{tri}} = 0.798/\sqrt{2} \) was obtained. To achieve this, we have done careful infinite volume and continuum limit extrapolations. In addition we offer a novel interpretation of \( \kappa_{\text{tri}} \), namely that it is also the value separating type-I and type-II behaviour.

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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 \( \phi \) coupled to a fluctuating mass-less gauge-field \( A \). The GL model in \( d \)-dimensions is defined by the functional integral

\[
Z = \int DA_i D\phi \exp(-S(A_i, \phi))
\]

\[
S = \int d^d x \left[ \frac{1}{4} F_{ij}^2 + |D_i \phi|^2 + m^2 |\phi|^2 + \lambda |\phi|^4 \right] \tag{1}
\]

where \( F_{ij} = \partial_i A_j - \partial_j A_i, D_i = \partial_i + i q A_i \), \( q \) is the charge coupling the condensate matter field to the fluctuating gauge-field, \( \lambda \) 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, phase transitions in liquid crystals, crystal melting, the quantum Hall effect and it is also used as an effective field theory describing phase transitions in the early Universe.

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 coefficients \( \alpha, \beta \) of the GL model by

\[
y = \frac{m^* c^2}{128\pi^2 \alpha_s^2 k_B T^2 \alpha}, \quad x = \frac{1}{8\pi \alpha_s \hbar} \left( \frac{m^* c}{\hbar} \right)^2 \beta = \kappa^2 \tag{2}
\]

where \( \alpha_s \) is the fine structure constant 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 Mehl it was shown that by ignoring spatial fluctuations in \( \phi \), and then integrating out the \( A \) field exactly, one gets a term \( |\phi|^3 \) in the effective \( \phi \) 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 \( \kappa \)), but even then it is very weak. For \( \kappa \ll 1 \) (type-I) the neglect of spatial variation in the matter field \( \phi \) is a reasonable approximation, whereas for \( \kappa \gg 1 \) (type-II) fluctuations in \( \phi \) must be taken into account. By doing a one-loop RG calculation using \( \varepsilon \)-expansion it was shown 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 \( \kappa \).

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 conven-
tional 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\cite{ma}. On the latter systems experiments can be carried out in the critical regime\cite{ma} and second order phase transitions are found. This contradicts the $\varepsilon$-expansion argument above, and presumably indicates a breakdown of the expansion for this gauge-field theory, since $\varepsilon = d - 1 = 1$.

In Ref.\cite{hal} it was shown, using duality arguments and Monte Carlo simulations, that the GL model should have a second order transition for large $\kappa$. However, what remains true is that deep in the type-I regime, the transition is first order. There should therefore be a tricritical point $\kappa = \kappa_{tri}$ where the transition changes order.

A first estimate for $\kappa_{tri}$ was obtained by Kleinert in Refs.\cite{klei,klei2} by developing a disorder theory formulation from which he calculated the value

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

analytically\cite{klei}. Subsequently\cite{klei3} 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 $\kappa_{tri}$, giving $\kappa_{tri} \approx 0.4/\sqrt{2}$. 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 $\kappa_{tri}$ 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\cite{klei,clei,clei2}.

The one-loop $\varepsilon$-expansion result of Halperin et al.\cite{hal} has subsequently been improved to two-loop order\cite{hal2} drastically reducing the value of $N_c$ to 32, but still $N_c > 2$. 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\cite{hal2}. From this latter work one can also get an estimate of the critical $\kappa$ from $\kappa^* = \sqrt{\hat{u} / 6\xi} \approx 0.62 / \sqrt{2}$. 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 $\kappa$, separating first and second order transitions exists, however a precise value remains to be determined.\cite{hal2}

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 $\kappa$ separating first and second order phase transitions coincides with the $\kappa$ separating type-I and type-II superconductors at $y_c$.

## II. The Order of the Transition

The model in Eq.\cite{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/symmetric does not refer to a breakdown of the local gauge symmetry present in Eq.\cite{1}. Elitzur’s theorem\cite{elitzur} 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 to fix the gauge\cite{33}. In this case a phase transition must be found either by using non-local order parameters or by looking for non-analytic behavior in local quantities\cite{33} as we have done. E.g. the quantity $\langle \vert \psi \rangle^2 \rangle$ 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 $\chi_{\vert \psi \rangle^2}$ will still have a peak.

In principle, we could therefore decide the order by looking for a jump in some local quantity as $\langle \vert \psi \rangle^2 \rangle$, 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.\cite{33}.

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\cite{33}.

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

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

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 the disordered phase. Near the tricritical value of $\kappa$ 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.

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\cite{4} of Lawrie and Sarbach\cite{3} 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

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

Right at the tricritical point the coefficients in front of both $|\phi|^2$ and $|\phi|^4$ 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 $\Delta |\phi|^2$ will vanish as

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

We will make use of the above scaling in section 11 to estimate $x_{\text{tri}}$. For further information about tricritical points, we refer to an extensive review by Lawrie and Sarbach.\cite{3}

In Fig. 2 we have assumed that the tricritical point separating first order 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 $\kappa_{\text{tri}} = 1/\sqrt{2}$ was not renormalized by fluctuations. We have not focused on the aspect of type-I/II superconductivity in our simulations, we will however argue that the overall structure of the phase diagram shown in Fig. 2 is correct in the vicinity of the tricritical point.

The microscopic difference between type-I and type-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 $\phi$ 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 $\kappa - \kappa_{\text{tri}}$, where $\kappa_{\text{tri}}$ is indeed to be identified with our tricritical value of $\kappa$.\cite{3} Using the dual formulation of the GL theory, it then becomes clear that $\kappa_{\text{tri}}$ is at the same time the value that separates first order 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\cite{37} we have calculated the fractal dimension of vortex loops, and found the scaling relation $\beta = \nu (d-D_{\text{H}})/2$, where $\beta$ is the order parameter exponent, $\nu$ is the correlation length exponent and $D_{\text{H}}$ is the fractal dimension of the loops. If

![Figure 1: A conjectured phase diagram in the $(x, y)$ plane in the vicinity of the tricritical point.](image)
where 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 $D_H \to d$, 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.

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 $(x_{xri}, y_{xri})$. 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 $x_{1/H} = 1/2$ 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

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

where $\beta_H$ so far is an arbitrary constant, Eq. 1 takes the form

$$Z = \int DA_i D\psi \exp(-S(A_i, \psi))$$

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

(7)

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

$$S = \beta_G \sum_{\bar{x},i<j} \frac{1}{2} F_{ij}^2 - \beta_H \sum_{\bar{x},i} \text{Re} \left( \psi^* U_i(\bar{x}) \psi(\bar{x} + \bar{i}) \right) + \sum_{\bar{x}} |\psi|^2 + \beta_R \sum_{\bar{x}} (|\psi|^2 - 1)^2.$$

(8)

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

The amplitude and gauge-invariant phase difference $\Delta = \arg(\psi^* U_i(\bar{x}) \psi(\bar{x} + \bar{i}))$ 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 $\Delta$ 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 ($\overline{MS}$) 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

$$y \to y - \frac{3.1759111(1 + 2x)}{2\pi} \beta_G$$

$$- \frac{(-4 + 8x - 8x^2)(\ln(6\beta_G) + 0.09) - 1.1 + 4.6x}{16\pi^2} + O(1/\beta_G).$$

(9)

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

$$\frac{\langle \phi^* \phi \rangle_{cont}}{q^2} = \frac{\beta_H \beta_G}{2} \langle \psi^* \psi \rangle_{latt}$$

$$- \frac{3.175911 \beta_G}{4\pi} - \frac{\log(6\beta_G) + 0.668}{8\pi^2} + O(1/\beta_G).$$

(10)

In Eq. 10 the first term comes from Eq. 5, 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 $y$, 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 $\xi$ 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 non-universal 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 [9] and gauge-fields. We have used periodic boundary conditions and non-compact gauge-fields without any gauge fixing. To reduce autocorrelation times we have added global updating of the amplitude and overrelaxation of the scalar field [10,11,12] 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) 2-3 overrelaxation “sweeps” updating both the amplitude and the phase of the scalar field. The acceptance ratio in the Metropolis steps is kept between 60-70% 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. [13,14,15].

We have performed simulations for the parameters in Table III. The simulations have been done in a hierarchical manner: For a given $a_q$ we have first kept $a_q$ and $N$ fixed, and simulated on typically three to eight $y$ values. The runs have been combined with Ferrenberg-Swendsen reweighting techniques, and a (pseudo)critical $y$ has been located by requiring that the reweighted histograms have two equally high peaks. Then the system size has been increased 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 state about ten times. Depending on system size and $x$-value (i.e. the strength of the first order transition) this resulted in about $10^5$ to $10^6$ 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 $5 \cdot 10^4$ CPU hours were used, corresponding to $\simeq 1.5 \cdot 10^{17}$ floating point operations.

VI. RESULTS

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

$$\overline{|\psi|^2} = \frac{1}{N^2} \sum_x |\psi(x)|^2$$

(11)

and histograms of this quantity constitute the raw data for most of the subsequent analysis [16]. The connection between continuum and lattice condensates is given by Eq. [15].

Histograms reweighted to the critical $y$-value are shown in Fig. 2. We have used two different methods to find $x_{tri}(a_q)$ 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 $\overline{|\psi|^2}$ to zero

The distance between the peaks of a histogram gives $\overline{\Delta |\psi|^2}(N)$, and by computing this for several different system sizes one can compute the infinite volume limit $\lim_{N \to \infty} \overline{\Delta |\psi|^2}$ of the discontinuity at the transition. Then one can (in principle) extrapolate to larger $x$ and find the value $x_{tri}$ where the discontinuity disappears. Results for $\lim_{N \to \infty} \overline{\Delta |\psi|^2}$ as a function of $x$ are shown in Fig. 2. For small $x$ the curves in Fig. 2 show a distinct positive curvature, but when approaching $x_{tri}$ we find that $\overline{\Delta |\psi|^2}$ vanishes as $\propto (x_{tri} - x)$, in accordance with mean-field theory, Eq. [27]. Also in the original attempt to locate $x_{tri}$ with Monte Carlo simulations [18] this extrapolation was done, however the extrapolation was done starting from quite small $x$ values, and the resulting $x_{tri}$ was much smaller than the one we calculate.

The extrapolated results for $x_{tri}$ are shown in Table IV. The values found should provide a reasonable upper limit.
a) $a_q = 0.5$

b) $a_q = 1.0$

c) $a_q = 2.0$

d) $a_q = 5.0$

FIG. 2: Normalized histograms $P(|\psi|^2)$ as a function of $|\psi|^2$ for a) $a_q = 0.5$, b) $a_q = 1.0$, c) $a_q = 2.0$, 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.

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

| $a_q$ | $x_{tri}$ (from $\Delta |\psi|^2$) | $x_{tri}$ (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                     |

for $x_{tri}(a_q)$.

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

It is also possible to study the height of the peaks in the histograms $P(|\psi|^2)_{\text{max}}$ relative to the minimum between them $P(|\psi|^2)_{\text{min}}$. This constitutes the best method of determining whether a transition is first order or not, but one cannot extrapolate to find $x_{tri}$. In Fig. 4 we show some typical results for $\Delta F(N) = \ln P_{\text{max}} - \ln P_{\text{min}}$ as 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 $N \geq 40$. This is expected since the histograms in Fig. 3 show a very pronounced double peak structure.

For larger $x$ this becomes less clear. Our estimates of $x_{tri}$ for the different lattice constants are given in Table II. The results are consistently somewhat below those found with method A and give a reasonable lower limit for $x_{tri}$.

C. Other methods

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

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

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 $\kappa_{tri}$

It is clear that it becomes increasingly difficult to obtain good estimates of $\kappa_{tri}(a_q)$ 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. 3, we show \( x_{tri}(a_q) \) found from extrapolation of \( \Delta |\psi|^2 \) to zero and from finite size scaling of \( \Delta F(N) \) as given in Table 1. A linear fit to the data gives \( \lim_{a_q \to 0} x_{tri}(a_q) = 0.287 \pm 0.004 \) 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 \( x_{tri}(a_q) \) increases considerably when we reduce \( a_q \) one cannot rule out other behaviors, as quadratic. From the “worst case scenario” shown by the dotted lines in the figure we get \( \lim_{a_q \to 0} x_{tri}(a_q) = 0.295 \pm 0.025 \). This in all likelihood gives a more realistic estimate of the error, and we therefore give our final estimate of \( \kappa_{tri} \) as \( \lim_{a_q \to 0} \kappa_{tri}(a_q) = (0.76 \pm 0.04)/\sqrt{2} \).
VI. 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 \( \kappa_{tr1} \approx 0.76 \pm 0.04 \). This is in remarkable agreement with the first estimate of \( \kappa_{tr1} \) obtained by Kleinert using a mean-field theory on the dual of the Ginzburg-Landau model, but differs almost by a factor of two from the subsequent early simulation results of Bartholomew.

The reason for the remarkable agreement with our result and those of Ref. 14 is that for small to intermediate values of \( \kappa \), 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. 13

The dual description of the Ginzburg-Landau model has recently met with considerable success in predicting the phase-transition of extreme type-II superconductors, even in magnetic fields. 14 We interpret the good agreement between our results and those of Ref. 14 as further support to the dual description of the Ginzburg-Landau model, now also in the intermediate-\( \kappa \) region.

We have also argued that this \( \kappa_{tr1} \) coincides with the \( \kappa \) separating type-I and type-II superconductivity. In the superconducting regime for \( \kappa \in (\kappa_{tr1}, 1/\sqrt{2}) \) 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 \( \kappa \) 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. 5.

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35 The fine structure constant is given by $\alpha_s = \frac{\mu_0 e^2}{4\pi}$, where $2e^*$ is the effective charge of a Cooper pair.
36 We acknowledge Prof. H. Kleinert for pointing out this formula to us.
37 In perturbation theory it is necessary to fix a gauge to avoid infinities from the infinite number of physically equivalent configurations. For simulations only the explicitly sampled configurations contribute, and no infinities arise. Finally the implementation on a parallel computer is simplest without gauge fixing.
38 The proportionality factor between $\Delta F$ and the cross-sectional area $L^{d-1}$ is the surface tension $\sigma$, which vanishes at $x_{\text{tr}}$, but due to the difficulty in getting proper $L^{d-1}$ scaling of $\Delta F$, we have not considered $\sigma$.
39 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 critical points which, in a suitably enlarged parameter space, may be found to meet here.
40 Note that in the London limit, with spatially constant amplitude, one cannot access the type-I regime. The 3DXY model coupled to a gauge-field is the dual of the 3DXY-model with no gauge-field fluctuations. The latter has a critical point corresponding to the 3DXY universality class, while the former recently has been shown explicitly to have a stable infrared charged fixed point. See J. Hove and A. Sudbø, Phys. Rev. Lett., 84, 3426 (2000).
41 We have used equal height histograms instead of equal weight. The reason for this is that, in particular for small systems, the histograms are quite asymmetric. Then the equal weight histograms are not well defined for weak first order transitions. Both methods should give the same results in the infinite volume limit, but the convergence rate may be different.
42 In addition to $|\psi|^2$ we have also studied other quantities, in particular
$$\mathcal{L} = \frac{1}{3N^3} \sum_{x,i} \cos (\arg [\psi^*(\vec{x})U_i(\vec{x})\psi(\vec{x} + \hat{i}))],$$
which varies between zero in the symmetric state and one in the broken state, quite similar to the more familiar 3DXY quantity $\langle \cos (\theta(x) - \theta(x + i)) \rangle$. However, the general picture is that the different observables give essentially the same information, and we have therefore focused mainly on Eq. [3], which has a well defined continuum limit.