Phase Transition in Complex $|\psi|^4$ Theory

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Motivated by recent claims for rather unconventional first-order phase transitions in the two- and three-dimensional complex $|\psi|^4$ theory in certain parameter ranges we performed Monte Carlo simulation studies of this model. From our results in two and three dimensions we can unambiguously conclude that there is *no* evidence for a first-order transition, provided the measure of field fluctuations is treated properly. The origin of the discrepancy is traced by comparative simulations reproducing the erroneous results and by a transfer-matrix study of the one-dimensional case.

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Scalar fields with n components and a fourth-order O(n)-symmetric quartic self-interaction are so far the best understood examples of systems, whose second-order phase transitions can be treated with field-theoretic techniques [1,2]. Perturbative calculations of critical exponents and amplitude ratios of the Ising, XY, Heisenberg, . . . spin models and the concept of universality relied heavily on this field-theoretic formulation. Universality ensures that spin models which describe only directional fluctuations show the same critical properties as scalar fields with $n \geq 2$ components, and the precise reason for this can easily be understood [3]. In particular, this equivalence holds for the superfluid phase transition which can be described either by a directional XY model or by an O(n)-symmetric scalar field theory, whose Hamiltonian is commonly expressed with a complex field $\psi(\vec{r}) = |\psi(\vec{r})|e^{i\phi(\vec{r})}$ in the Ginzburg-Landau form as

$$H[\psi] = \int d^d r \left[\alpha|\psi|^2 + \frac{b}{2}|\psi|^4 + \frac{\gamma}{2}|\nabla\psi|^2 \right], \gamma > 0. \quad (1)$$

It came therefore as a surprise when, on the basis of an approximate variational approach to the two-component Ginzburg-Landau model, Curty and Beck [4] recently predicted for certain parameter ranges the possibility of first-order phase transitions induced by phase fluctuations. Being not so credible to start with, in several papers [5–9] this uncontrolled quasianalytical [10] approximation was tested by Monte Carlo simulations. As a result the rather unconventional claim by Curty and Beck [4] was apparently confirmed numerically. If true, these findings would have an enormous impact on the theoretical description of many related systems such as superfluid helium, superconductors, certain liquid crystals and possibly even the electroweak standard model of elementary particle physics [11,12].

Although it came as a surprise, the result is not completely nonsensical in view of an old observation in Ref. [13], that an appropriately mixed action of the purely directional XY type can have first-order transitions. However, this was caused by the generation of a negative coefficient of the effective quartic interaction from fluctuation, whereas it was hard to see how such a sign change could be achieved in (1).

In view of the potentially important implications for a broad variety of different fields we report here the results of independent Monte Carlo simulations of the model (1) in two and three dimensions to show that the claim of phase-fluctuation induced first-order transitions in Refs. [5–9] is incorrect. The source for the wrong result is pointed out. We also give a further argument in favor of our result by a transfer-matrix study of the one-dimensional complex Ginzburg-Landau chain. Our results clearly support the conventional opinion that the transition in the Ginzburg-Landau model as in the parametrization of Curty and Beck [4] is of second-order. As often noticed [14], variational approximations are not a reliable tool to determine the order of a transition, and the same thing is true for the approximation employed by Ref. [4].

In order to carry out the Monte Carlo simulations we put the model (1) on a d-dimensional hypercubic lattice with spacing a. Adopting the notation of Ref. [4] we normalize the Hamiltonian by setting $\tilde{\psi} = \psi/\sqrt{(|\alpha|/b)}$, $\tilde{u} = \vec{r}/\xi$, where $\xi^2 = \gamma/|\alpha|$ is the mean-field correlation length at zero temperature. The normalized lattice Hamiltonian is thus given by

$$H[\tilde{\psi}] = k_B \tilde{V}_0 \sum_{n=1}^{N} \left[\frac{\tilde{\sigma}}{2}(|\tilde{\psi}_n|^2 - 1)^2 + \frac{1}{2}\sum_{\mu=1}^{d} |\tilde{\psi}_n - \tilde{\psi}_{n+\mu}|^2 \right], \quad (2)$$

where we have removed a constant term, μ denotes the unit vector along the μ axes, and $N = L^d$ is the total number of sites. Only two parameters remain,

$$\tilde{\sigma} = \frac{a^2}{\xi^2}, \qquad \tilde{V}_0 = \frac{1}{k_B}\frac{|\alpha|}{b}\gamma a^{d-2}, \quad (3)$$

where furthermore $\tilde{V}_0$ can be used to set the scale of the (dimensionless) temperature. The partition function Z is

$$Z = \int D\psi D\bar{\psi} e^{-H/\tilde{T}}, \tag{4}$$

where the reduced temperature is defined as $\tilde{T} = T/\tilde{V}_0$ and $\int D\psi D\bar{\psi}$ stands short for summing over all possible complex field configurations.

In our simulations described in detail below we have measured among other quantities the energy density $e = \langle H\rangle/N$, the specific heat $c_v = (\langle H^2\rangle - \langle H\rangle^2)/N$, and in particular, the mean square amplitude

$$\langle|\tilde{\psi}|^2\rangle = \frac{1}{N}\left\langle \sum_{n=1}^{N} |\tilde{\psi}_n|^2 \right\rangle, \tag{5}$$

which will serve as the most relevant quantity for comparison with previous work [4–9]. For further comparison and in order to determine the critical temperature, the helicity modulus,

$$\begin{aligned}\Gamma_\mu = &\frac{1}{N}\left\langle \sum_{n=1}^{N} |\tilde{\psi}_n||\tilde{\psi}_{n+\mu}| \cos(\phi_n - \phi_{n+\mu}) \right\rangle \\ &- \frac{1}{N\tilde{T}}\left\langle \left[\sum_{n=1}^{N} |\tilde{\psi}_n||\tilde{\psi}_{n+\mu}| \sin(\phi_n - \phi_{n+\mu}) \right]^2 \right\rangle,\end{aligned} \tag{6}$$

was also computed. Notice that the helicity modulus Γ_μ is a direct measure of the phase correlations in the direction of μ. In the infinite-volume limit, Γ_μ is zero above T_c and different from zero below T_c. For notational simplicity we will omit in the rest of the Letter the tilde on ψ, σ, and T.

Let us now turn to the description of the Monte Carlo update procedures used by us. Since we suspected from the outset some flaws in the previous numerical results, we started with the most straightforward (but most inefficient) algorithm known since the early days of Monte Carlo simulations: The standard Metropolis algorithm [15]. Here the complex field ψ_n is decomposed in its Cartesian components, $\psi_n = \psi_{x,n} + i\psi_{y,n}$. For each lattice site a random update proposal for the two components is made, e.g., $\psi_{x,n} \to \psi_{x,n} + \delta\psi_{x,n}$ with $\delta\psi_{x,n} \in [-\Delta, \Delta]$, and in the standard fashion accepted or rejected according to the energy change δH. The parameter Δ is usually chosen such as to give an acceptance rate of about 50%, but other choices are permissible and may even result in a better performance of the algorithm (in terms of autocorrelation times). All this is standard [16] and guarantees in a straightforward manner that the complex measure $D\psi D\bar{\psi}$ in the partition function (4) is treated properly.

The well-known drawback of this algorithm is its critical slowing down (large autocorrelations) in the vicinity of a continuous phase transition [16], leading to large statistical errors for a fixed computer budget. To improve the accuracy of our data we therefore employed the single-cluster algorithm [17] to update the direction of the field [18], similar to simulations of the XY spin model [19]. The modulus of ψ is updated again with a Metropolis algorithm. Here some care is necessary to treat the measure in (4) properly (see below). Per measurement we performed one sweep with the Metropolis algorithm and m single-cluster updates. For the 3D model the number of cluster updates was chosen roughly proportional to the linear lattice size L, a standard choice as suggested by a simple finite-size scaling analysis. For $L = 15$ we thermalized with 500 to 1000 sweeps and averaged the measurements over 10 000 sweeps.

All error bars are computed with the Jackknife method [20]. In the following, we show only the more extensive and accurate data set of the cluster simulations, but we tested in many representative cases that the Metropolis simulations coincide within error bars. In Fig. 1(a) the mean square amplitude $\langle|\psi|^2\rangle$ for the 3D model is shown as a function of T for different values of the parameter σ. We see a smooth variation with temperature and definitely *no* indication of a first-order phase transition as claimed in Refs. [5–9]. For precisely the same set of parameters and lattice size L the simulations of Refs. [5,9] yielded results which are consistent within error bars with our Fig. 1(b)

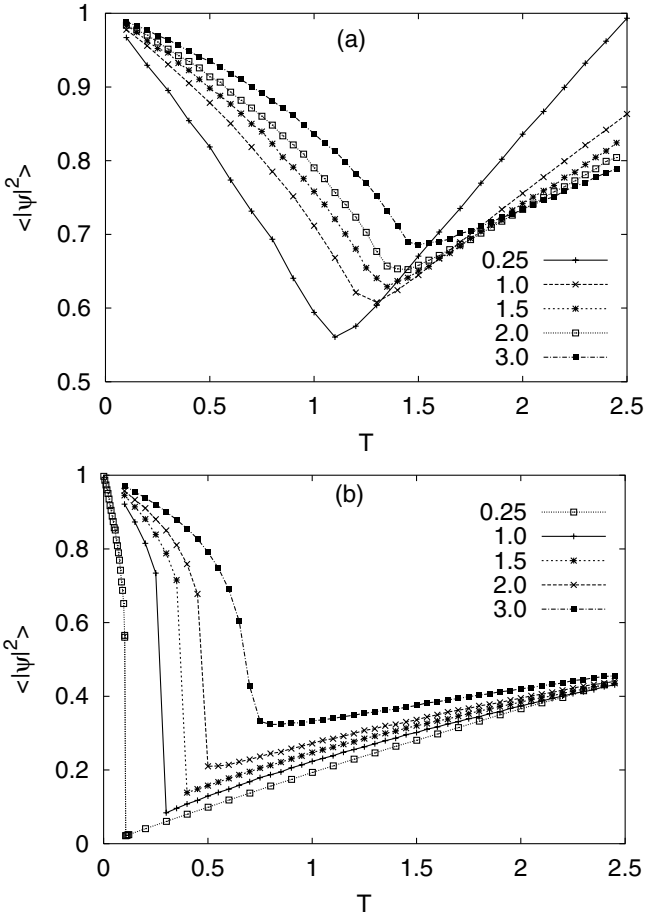

FIG. 1. (a) Mean square amplitude of the 3D Ginzburg-Landau model on a 15^3 cubic lattice for different values of the parameter $\sigma = 0.25, \ldots, 3.0$. (b) The same quantities using the *incorrect* Jacobian in the polar coordinates representation (7) (see text).

and which, in fact, look indicative of first-order transitions, at least for small values of σ.

What is the reason for this pronounced discrepancy? The disagreement is the result of an incorrect treatment of the Jacobian which emerges from the complex measure in (4) when transforming the field representation. If we decompose the field ψ_n in polar coordinates, $\psi_n = R_n[\cos(\phi_n), \sin(\phi_n)]$, and update in the simulations the modulus $R_n = |\psi_n|$ and the angle ϕ_n, then we have to rewrite the partition function (4) as

$$Z = \int_0^{2\pi} D\phi \int_0^{\infty} R\, DR e^{-H/T}, \tag{7}$$

where $R \equiv \prod_{n=1}^{N} R_n$ is the Jacobian of this transformation. While mathematically indeed trivial (and properly taken into account in Ref. [4]), this fact may easily be overlooked when coding the update proposals for the modulus and angle in the Monte Carlo simulation program. In fact, if we ignore the Jacobian and simulate the model (7) (erroneously) without the R factor, then we obtain the results displayed in Fig. 1(b). As already mentioned above these results reproduce [21] those in Refs. [5,9], and from this data one would indeed conclude evidence for a first-order phase transition when σ is small. With the correct measure, on the other hand, we have checked that *no* first-order signal shows up down to $\sigma = 0.01$. The same conclusion can be drawn by looking at other quantities such as the helicity modulus (6). Technically speaking, in the simulations the erroneous omission of the R factor results from the implicit assumption of a uniform measure not only for the angles $\phi_n \in (0, 2\pi)$ (correct), but also for the modulus $R_n \in (0, \infty)$ (incorrect).

To treat the measure in Eq. (7) properly one can either use the identity $R\, DR = DR^2/2$ and update the squared moduli $R_n^2 = |\psi_n|^2$ according to a uniform measure, or one can introduce an effective Hamiltonian,

$$H_{\text{eff}} = H - T\kappa \sum_{n=1}^{N} \log R_n, \tag{8}$$

with $\kappa \equiv 1$ and work directly with a uniform measure for R_n. The omission of the R factor in (7) corresponds to setting $\kappa = 0$. It is well known [11] that the nodes $R_n = 0$ correspond to core regions of vortices in the dual formulation of the model. The Jacobian factor R (or equivalently the term $-\sum \log R_n$ in H_{eff}) tends to suppress field configurations with many nodes $R_n = 0$. If the R factor is omitted, the number of nodes and hence vortices is relatively enhanced. It is thus at least qualitatively plausible that in this case a discontinuous, first-order "freezing transition" to a vortex dominated phase can occur, as is suggested by a similar mechanism for the XY model [11,22] and defect models of melting [23,24].

In order to check our update algorithm, we performed further simulations of a one-dimensional chain with the Hamiltonian defined in Eq. (2) and compared the results with (numerically exact) transfer-matrix calculations for the same model. We used a chain of length $L = 400$ with periodic boundary conditions. In the Monte Carlo simulations we thermalized with 5000 sweeps and averaged over 5000 sweeps for different values of σ. To determine the quantities for the chain by transfer-matrix calculations we extended the method described in Refs. [25–27] to a two-component field. As is demonstrated in Fig. 2, the two methods, proper Monte Carlo simulations and transfer-matrix calculations, give indeed the same results (the error bars on the Monte Carlo data are smaller than the symbols). Also shown are the results obtained with the incorrect update procedure (i.e., ignoring the R factor coming from the Jacobian)—the outcome of this final test is indisputable.

We also performed simulations in two dimensions and found the same error in the results given in Refs. [6–8], i.e., in particular, we found again *no* evidence for a first-order phase transition.

To summarize, the possibility of a phase-fluctuation induced first-order phase transition in the Ginzburg-Landau model as suggested by approximate variational calculations by Curty and Beck [4] cannot be confirmed by our numerical simulations. Contrary claims in previous numerical work [5–9] in two and three dimensions are incorrect due to the omission of the Jacobian factor $R = \prod_{n=1}^{N} R_n$, appearing when transforming the complex field integration to polar coordinates $\psi_n = R_n[\cos(\phi_n), \sin(\phi_n)]$. By exponentiating the Jacobian factor R, it becomes qualitatively clear that its omission tends to enhance the condensation of vortices which can trigger the erroneously claimed first-order phase transitions.

Turning the arguments around, our results suggest that the Ginzburg-Landau model can be modified to undergo a first-order transition in a way similar to Ref. [13] by varying the coefficient κ of the $-\sum \log R_n$ term in the effective Hamiltonian (8). As in Ref. [13] this can be understood by

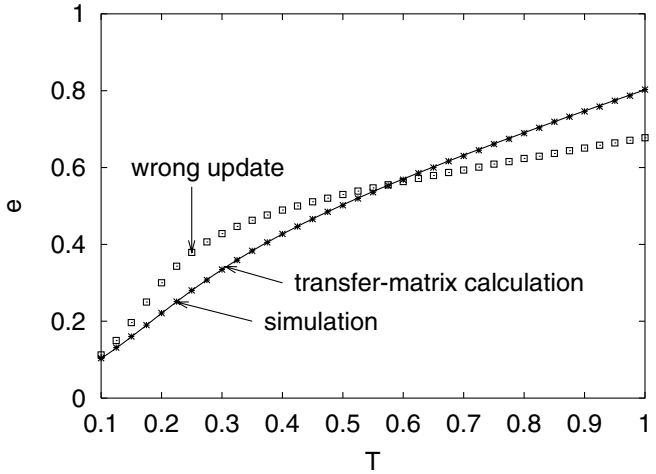

FIG. 2. Energy density of the one-dimensional Ginzburg-Landau chain of length $L = 400$ for $\sigma = 1$.

a duality argument. The extra term reduces the ratio of core energies of vortex lines of vorticity 2 versus those of vorticity 1, and this leads to the same type of transition as observed in defect melting of crystals. A study of the tricritical point as a function of κ would be an interesting future project.

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