GENERALIZED COMPLEX $|\psi|^4$ MODEL*

Elmar Bittner† and Wolfhard Janke‡

Institut für Theoretische Physik, Universität Leipzig
Augustusplatz 10/11, 04109 Leipzig, Germany

(Received August 18, 2003)

We study the complex $|\psi|^4$ theory in three dimensions and compare our numerical results with a recently proposed mean-field like approximation. The mean-field result, which predicts a first-order phase transition in parts of the phase diagram, cannot be confirmed. To get a closer look inside this discrepancy, we introduce a generalized Hamiltonian with an additional fugacity term. With this modification we can show that the complex $|\psi|^4$ theory can indeed be tuned to undergo a first-order phase transition by varying the strength of the new term in the generalized Hamiltonian.

PACS numbers: 02.70.Lq, 64.60.–i, 74.20.De

1. Introduction

Since long the Ginzburg–Landau model has been considered as paradigm for studying critical phenomena using field-theoretic techniques [1]. 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 [2]. Even though the spin models contain only directional fluctuations, while for n-component Ginzburg–Landau fields with $n \geq 2$ directional and size fluctuations seem to be equally important, the two descriptions are completely equivalent. This equivalence can easily be proved for superfluids with $n = 2$ where the spin model reduces to an XY model [3]. Therefore it appeared 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. In several papers [5–9] this quasi-analytical [10] prediction was tested by

* Presented at the Workshop on Random Geometry, Kraków, Poland, May 15–17, 2003.

† e-mail: Elmar.Bittner@itp.uni-leipzig.de
‡ e-mail: Wolfhard.Janke@itp.uni-leipzig.de

Monte Carlo simulations and, as the main result, 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].

In view of these potentially important implications for a broad variety of different fields we performed independent Monte Carlo simulations of this model in two and three dimensions [13] in order to test whether the claim of phase fluctuation induced first-order transitions is a real effect or not. As the main message of our study: it is not! Rather, our results clearly support the conventional opinion that the nature of the transition in the parameterization of the Ginzburg–Landau model used by Curty and Beck [4] is of second order. In turn this implies, of course, that the variational approximation employed in Ref. [4] is less reliable than originally thought in view of the apparent numerical confirmations. As we pointed out in Ref. [13], the complex $|\psi|^4$ model can be modified to undergo a first-order transition by adding an additional fugacity term. In this work we study this model in three dimensions by means of Monte Carlo simulations, with particular emphasis placed on the order of the transitions as a function of the new fugacity term.

The remainder of the paper is organized as follows. In Sec. 2 we first recall the definition of the model and the observables. We then discuss the simulation techniques and present the results of our simulations in Sec. 3. In Sec. 4 we conclude with a brief summary of the main results.

2. Model and observables

Following the standard two-component Ginzburg–Landau theory, we define the Hamiltonian

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

where $\psi(\vec{r}) = |\psi(\vec{r})|\mathrm{e}^{i\phi(\vec{r})}$ is a complex field, and α, b and γ are coefficients independent of the temperature derived from a microscopic model. 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 $\tilde{\psi} = \psi/\sqrt{(|\alpha|/b)}$ and $\vec{u} = \vec{r}/\xi$, where $\xi^2 = \gamma/|\alpha|$ is the mean-field correlation length at zero temperature. The normalized lattice Hamiltonian is thus given by

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

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,

$$\tilde{\sigma} = \frac{a^2}{\xi^2}, \quad \tilde{V}_0 = \frac{1}{k_{\rm B}} \frac{|\alpha|}{b} \gamma a^{d-2} \ , \tag{3}$$

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

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

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

In Ref. [13] we have shown that the disagreement mentioned above is caused by an incorrect treatment of the Jacobian which emerges from the complex measure in (4) when transforming the field representation to polar coordinates, $\tilde{\psi}_n = R_n(\cos(\phi_n), \sin(\phi_n))$. When updating in the simulations the modulus $R_n = |\tilde{\psi}_n|$ and the angle ϕ_n, we have to rewrite the partition function (4) as

$$Z = \int_0^{2\pi} D\phi \int_0^{\infty} RDR \mathrm{e}^{-H/\tilde{T}} \ , \tag{5}$$

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]), the fact that the integration measure for R_n is *non-uniform* may easily be overlooked when coding the actual update proposals for the modulus in the Monte Carlo simulation program. In fact, if we ignore the Jacobian and simulate the model (5) (erroneously) without the R-factor, then we obtain a completely different behaviour than with the proper integration measure, see Fig. 1. As already mentioned above these results reproduce [14] 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 $\sigma = 0.01$.

To treat the measure in Eq. (5) properly one can either use the identity $RDR = DR^2/2^N$ and update the squared moduli $R_n^2 = |\tilde{\psi}_n|^2$ according to a *uniform* measure, or one can introduce an effective Hamiltonian,

$$H_{\rm eff} = H - \tilde{T}\kappa \sum_{n=1}^{N} \log R_n \ , \tag{6}$$

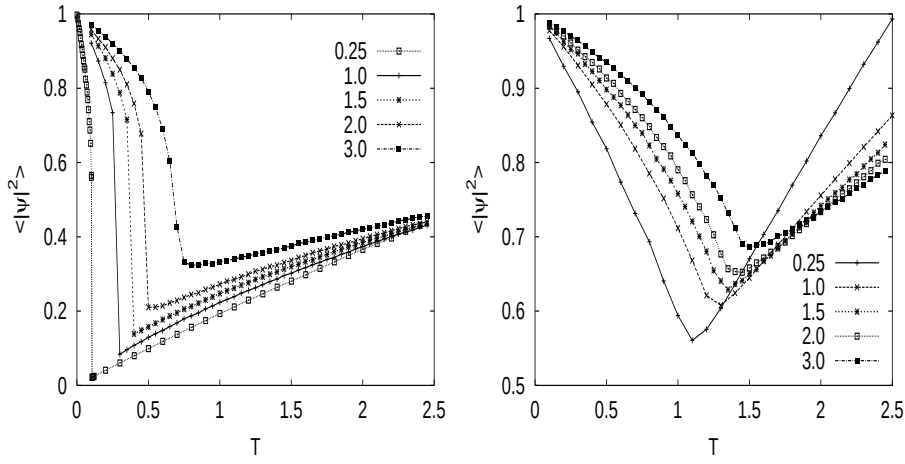

Fig. 1. Left plot: Mean square amplitude of the 3D Ginzburg–Landau model on a 15^3 cubic lattice for different values of the parameter $\sigma = 0.25, \ldots, 3.0$, using the *incorrect* Jacobian in the polar coordinates representation (5) (see text). Right plot: The same quantities with the proper integration measure.

with $\kappa \equiv 1$ and work directly with a *uniform* measure for R_n. The omission of the R-factor in (5) corresponds to setting $\kappa = 0$. It is well known [11] that the nodes $R_n = 0$ correlate with core regions of vortices in the dual formulation of the model. The Jacobian factor R (or equivalently the term $-\sum \log R_n$ in $H_{\rm eff}$) 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, 15] and defect models of melting [16, 17].

In our simulations of the three-dimensional (3D) generalized Ginzburg–Landau model (6) described in detail in the next section 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

$$\langle |\tilde{\psi}|^2 \rangle = \frac{1}{N} \sum_{n=1}^{N} \langle |\tilde{\psi}_n|^2 \rangle \ , \tag{7}$$

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,

$$\begin{aligned} \Gamma_\mu &= \frac{1}{N}\left\langle \sum_{n=1}^{N} |\tilde{\psi}_n||\tilde{\psi}_{n+\mu}| \cos(\phi_n - \phi_{n+\mu}) \right\rangle \\ &\quad -\frac{1}{N\tilde{T}}\left\langle \left[\sum_{n=1}^{N} |\tilde{\psi}_n||\tilde{\psi}_{n+\mu}| \sin(\phi_n - \phi_{n+\mu})\right]^2 \right\rangle \ , \end{aligned} \tag{8}$$

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. To complete the picture we furthermore measured the vortex-line density v. The standard procedure to calculate the vorticity of each plaquette is by considering the quantity

$$m_{*p} = \frac{1}{2\pi}\left([\phi_1 - \phi_2]_{2\pi} + [\phi_2 - \phi_3]_{2\pi} + [\phi_3 - \phi_4]_{2\pi} + [\phi_4 - \phi_1]_{2\pi}\right) \ , \tag{9}$$

where $[\alpha]_{2\pi}$ stands for α modulo 2π: $[\alpha]_{2\pi} = \alpha + 2\pi n$, with n an integer such that $\alpha + 2\pi n \in (-\pi, \pi]$, hence $m_{*p} = n_{12} + n_{23} + n_{34} + n_{41}$. The symbol $*p$ denotes the link dual to a given plaquette p. If $m_{*p} \neq 0$, there exists a vortex line which is assigned to the object dual to the given plaquette. The vortex "charge" m_{*p} can take three values: $0, \pm 1$ (the values ± 2 have a negligible probability). The vortex-line density is defined as

$$v = \frac{1}{N}\sum_{*p} |m_{*p}| \ . \tag{10}$$

We further analyzed the Binder cumulant,

$$U = \frac{\langle (\vec{m}^2)^2 \rangle}{\langle \vec{m}^2 \rangle^2} \ , \tag{11}$$

where

$$\vec{m} = \frac{1}{N}\sum_{n=1}^{N} \tilde{\psi}_n \tag{12}$$

is the magnetization per lattice site of a given configuration. For notational simplicity we will omit in the rest of the paper the tilde on ψ, σ, and T.

3. Simulation techniques and results

Let us now turn to the description of the Monte Carlo update procedures used by us. We employed the single-cluster algorithm [18] to update the direction of the field [19], similar to simulations of the XY spin model [20]. The modulus of ψ is updated with a Metropolis algorithm [21,22]. Here some care is necessary to treat the measure in (4) or (5) properly (see [13]). Per measurement we performed one sweep with the Metropolis algorithm and m single-cluster updates. For all simulations the number of cluster updates was chosen roughly proportional to the linear lattice size L, a standard choice for 3D systems as suggested by a simple finite-size scaling analysis. We performed simulations for lattices with linear lattice size $L = 10, 15$, 20, and 30, respectively, subject to periodic boundary conditions. For each simulation point we thermalized with 500 to 1 000 sweeps and averaged the measurements over 10 000 sweeps. All error bars are computed with the Jackknife method [23].

First we investigated the size dependence of the model by simulating different lattice sizes for $\kappa = 0$ and $\kappa = 1$ at fixed $\sigma = 0.25$. As can be seen in Fig. 2, there is only a small dependence on the variation of the lattice size for the energy and the mean square amplitude. The same conclusion can be drawn by looking at other quantities such as the helicity modulus (8) and the vortex-line density (10), see Fig. 3. On the basis of these results, we do not expect a change of the behaviour for significant larger lattices, therefore we used moderate lattice sizes for our further investigations.

The remarkable difference between the curves for the different values of κ leads us to the question of the order of the phase transitions. One possible method to distinguish between phase transitions of first and second order is to look at histograms of the energy or magnetization close to the transition point [24]. For $\sigma = 0.25$ and $\kappa = 0$ we find a double-peak structure for the energy and the mean square amplitude as well for the mean modulus $\overline{|\psi|} = \frac{1}{N}\sum_{n=1}^{N}|\psi_n|$ shown in Fig. 4. The pronounced dip over more than 20 orders of magnitude is a clear indication for two coexisting phases, therefore we conclude that for $\kappa = 0$ the model undergoes a first-order phase transition. For $\kappa = 1$, on the other hand, we find a single-peak structure for all three quantities, see Fig. 4. These results support the conventional opinion that the complex $|\psi|^4$ model undergoes a second-order phase transition.

To get a more precise idea of the κ dependence of the generalized model (6) and especially to determine the phase transition line, we performed simulations for $\kappa = 0$ to 1 in steps of 0.1 and additionally $\kappa = 0.85$ and 0.95 at fixed $\sigma = 0.25$. In Fig. 5 we show for all values of κ the mean square amplitudes as a function of the temperature which indicate that there is indeed a region with first-order phase transitions (κ small) and another one

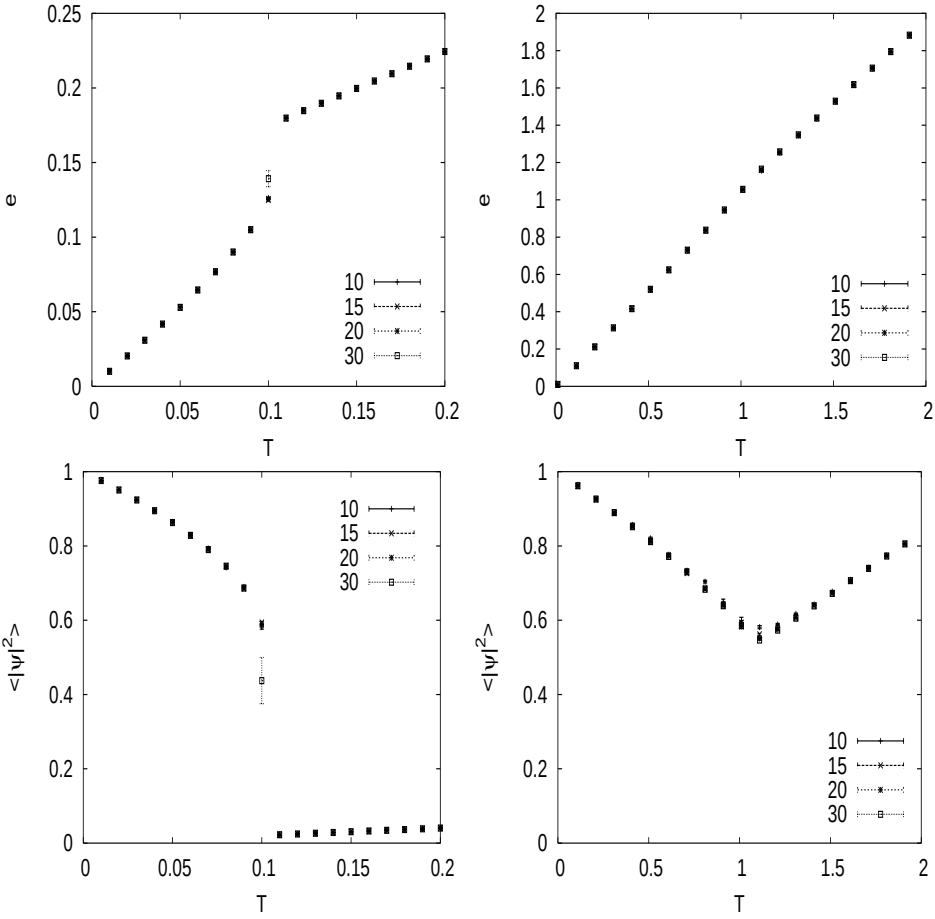

Fig. 2. Left plots: Energy density e and mean square amplitude $\langle|\psi|^2\rangle$ on various cubic lattices with $\sigma = 0.25$ and $\kappa = 0$. Right plots: The same quantities with $\kappa = 1$.

with second-order phase transitions ($\kappa \to 1$). In order to locate and check the order of the phase transitions we used for various κ values a variant of the multicanonical scheme [25, 26]. Instead of flattening the histogram of the energy or magnetization, here we sampled the system with weight factors for the mean modulus. With this simulation technique we overcome the difficulty of sampling the rare events between the two peaks of the modulus distribution close to a first-order phase transition, *cf.* Fig. 4. Moreover, with this simulation scheme we can examine a wide range in the parameter space with only one simulation by applying reweighting techniques. For several values of κ in the first-order region the transition point was then estimated

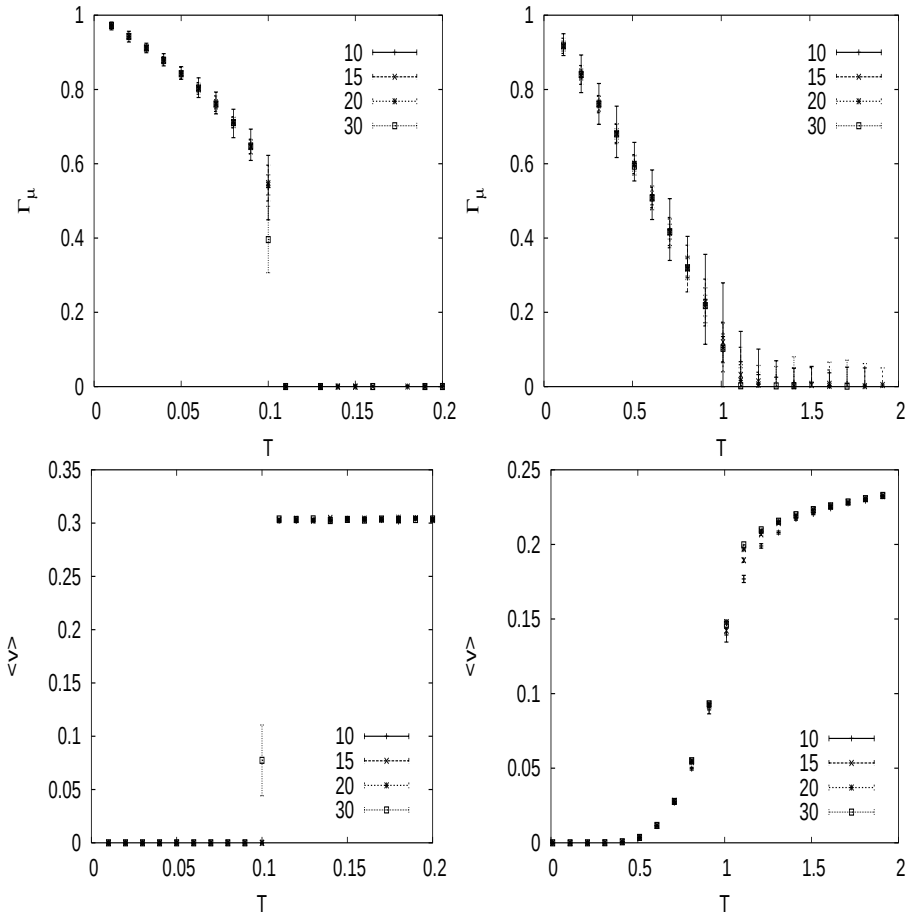

Fig. 3. Left plots: Helicity modulus Γ_μ and vortex-line density $\langle v \rangle$ on various cubic lattices with $\sigma = 0.25$ and $\kappa = 0$. Right plots: The same quantities with $\kappa = 1$.

by reweighting the distribution for the modulus to the temperature T_0 where the two peaks are of equal height. In the region of second-order transitions we used single-cluster updates combined with the Metropolis algorithm and found the location of the phase transition by looking at the crossing point of the Binder parameter for different lattices sizes L. In the right plot of Fig. 5 we show a preliminary phase diagram for $\sigma = 0.25$, where the boxes in the plot mark the transition points we have found. The tricritical point is roughly estimated to occur around $\kappa \approx 0.8$. Its precise location has not yet been determined; this will be left for an interesting, albeit technically rather involved future project.

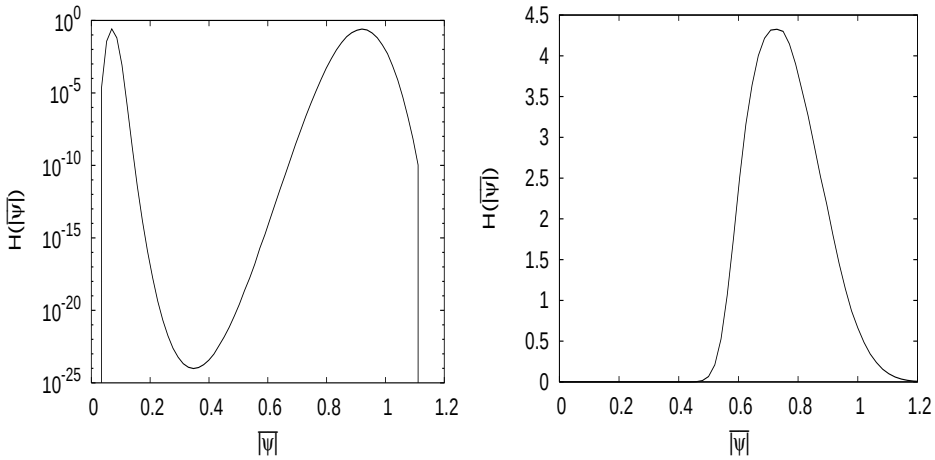

Fig. 4. Left plot: Histogram of the mean modulus $\overline{|\psi|}$ on a 4^3 lattice for $\sigma = 0.25$ and $\kappa = 0$ at the temperature $T_0 \approx 0.0572$ where both maxima are of equal height. Right plot: Histogram for the same quantity and lattice size for $\sigma = 0.25$ and $\kappa = 1$ at $T = 1.1$ close to the phase transition.

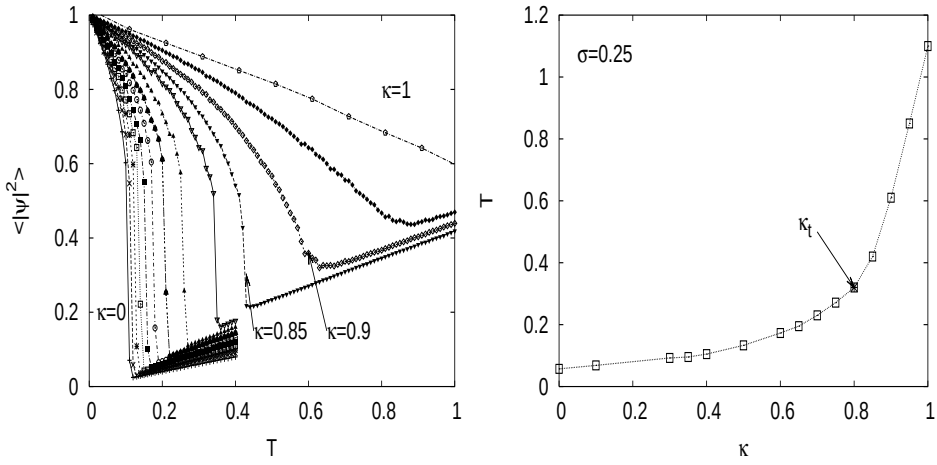

Fig. 5. Left plot: κ dependence of the mean square amplitude $\langle|\psi|^2\rangle$ as a function of the temperature on a 15^3 lattice for $\sigma = 0.25$. Right plot: Phase diagram of the generalized complex $|\psi|^4$ model for $\sigma = 0.25$. The transitions for $\kappa < \kappa_t$ are of first order, and the transitions for $\kappa > \kappa_t$ are of second order. The point κ_t at the intersection of these two lines is the tricritical point.

4. Summary

The possibility of a phase fluctuation induced first-order phase transition in the standard Ginzburg–Landau model as suggested by approximate variational calculations by Curty and Beck [4] cannot be confirmed by our numerical simulations. Instead of this we show that the three-dimensional Ginzburg–Landau model can be modified to undergo a first-order transition in a way similar to Ref. [27] by varying the coefficient κ of an additional $-\sum \log R_n$ term in the generalized Hamiltonian (6). As in Ref. [27] this can be understood by duality arguments. The extra term reduces the ratio of core energies of vortex lines of vorticity two versus those of vorticity one, and this leads to the same type of transition as observed in defect melting of crystals. We presented a first sketch of the phase diagram of the generalized complex $|\psi|^4$ model in the $\kappa - T$ plane and located roughly the tricritical point for one value of the parameter σ. The precise determination of the tricritical point and a study of the tricritical line as a function of κ and σ would be an interesting future project.

E.B. thanks the EU-Network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity" for a postdoctoral grant.

REFERENCES

[1] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, 3rd ed., Clarendon Press, Oxford 1996.

[2] H. Kleinert, V. Schulte-Frohlinde, *Critical Properties of* Φ^4*-Theories*, World Scientific, Singapore 2001.

[3] H. Kleinert, *Phys. Rev. Lett.* **84**, 286 (2000).

[4] P. Curty, H. Beck, *Phys. Rev. Lett.* **85**, 796 (2000).

[5] P. Curty, H. Beck, `cond-mat/0010084`.

[6] H. Fort, hep-th/0010070.

[7] G. Alvarez, H. Fort, *Phys. Rev.* **B63**, 132504 (2001).

[8] G. Alvarez, H. Fort, *Phys. Lett.* **A282**, 399 (2001).

[9] G. Alvarez, H. Fort, *Phys. Rev.* **B64**, 092506 (2001).

[10] The method of Ref. [4] uses XY model data as input.

[11] H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I: *Superflow and Vortex Lines*, World Scientific, Singapore 1989.

[12] V.M. Loktev, R.M. Quick, S.G. Sharapov, *Phys. Rep.* **349**, 1 (2001).

[13] E. Bittner, W. Janke, *Phys. Rev. Lett.* **89**, 130201 (2002).

[14] There is another difference between our update and the update described in the papers [5,9], namely that we do *not* restrict the modulus of the field to a finite interval. This can cause further systematic deviations but we explicitly checked that this is not crucial here.

[15] P. Minnhagen, M. Wallin, *Phys. Rev.* **B36**, 5620 (1987); G. Zhang, H. Chen, X. Wu, *Phys. Rev.* **B48**, 12304 (1993); D.Yu. Irz, V.N. Ryzhov, E.E. Tareyeva, *Phys. Rev.* **B54**, 3051 (1996).

[16] H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. II: *Stresses and Defects*, World Scientific, Singapore 1989.

[17] W. Janke, Int. J. Theor. Phys. **29**, 1251 (1990).

[18] U. Wolff, *Phys. Rev. Lett.* **62**, 361 (1989); *Nucl. Phys.* **B322**, 759 (1989).

[19] M. Hasenbusch, T. Török, *J. Phys. A* **32**, 6361 (1999).

[20] W. Janke, *Phys. Lett.* **A148**, 306 (1990).

[21] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, E. Teller, *J. Chem. Phys.* **21**, 1087 (1953).

[22] W. Janke, *Mathematics and Computers in Simulations* **47**, 329 (1998); and in: *Computational Physics: Selected Methods — Simple Exercises — Serious Applications*, eds. K.H. Hoffmann and M. Schreiber, Springer, Berlin 1996, p. 10.

[23] B. Efron, *The Jackknife, the Bootstrap and Other Resampling Plans*, Society for Industrial and Applied Mathematics [SIAM], Philadelphia 1982.

[24] W. Janke, *First-Order Phase Transitions*, to appear in: *Computer Simulations of Surfaces and Interfaces*, NATO Advanced Study Institute, Albena, Bulgaria, September 2002, eds. D.P. Landau, A. Milchev, B. Dünweg, Kluwer, Dordrecht, 2003, in print.

[25] B.A. Berg, T. Neuhaus, *Phys. Lett.* **B267**, 249 (1991); *Phys. Rev. Lett.* **68**, 9 (1992).

[26] U. Hansmann, B.A. Berg, T. Neuhaus, *Int. J. Mod. Phys.* **C3**, 1155 (1992).

[27] W. Janke, H. Kleinert, *Nucl. Phys.* **B270**, 399 (1986).