Phase Diagram of a Generalized $|\psi|^4$ model in two and three dimensions

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Complex $|\psi|^4$ Model

- The Hamiltonian according to Ginzburg-Landau theory

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

with $\psi(\vec{r}) = |\psi(\vec{r})| e^{i\phi(\vec{r})}$, and the temperature independent coefficients α, b and γ.

- On a d-dimensional hypercubic lattice with spacing a, and adopting the notation of Ref. [1]
($\tilde{\psi} = \psi / \sqrt{(|\alpha|/b)}, \vec{u} = \vec{r}/\xi$, with $\xi^2 = \gamma/|\alpha|$)

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

Only two parameters remain:
$\tilde{\sigma} = a^2/\xi^2, \quad \tilde{V}_0 = \frac{1}{k_B} \frac{|\alpha|}{b} \gamma a^{d-2}$.

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

The partition function is

$$Z = \int D\psi D\bar{\psi} e^{-H/\tilde{T}} = \int D\mathcal{R} D\phi e^{-(H-\tilde{T}\sum \log \mathcal{R})/\tilde{T}} \ ,$$

with $\tilde{T} = T/\tilde{V}_0$ and $\mathcal{R} = |\tilde{\psi}|$.

We can rewrite the Hamiltonian

$$H[R,\phi] = (H_R + \sum_{i=1}^{N} R_i^2 f_i)$$

where

$$f_i = \sum_{j=1}^{d} [1 - \cos(\phi_i - \phi_j)]$$

and

$$H_R = \sum_{i=1}^{N} [\sigma(R_i^2 + R_i^4/2) + (\nabla R_i)^2/2] \ .$$

This leads to the effective Hamiltonian H_{eff}

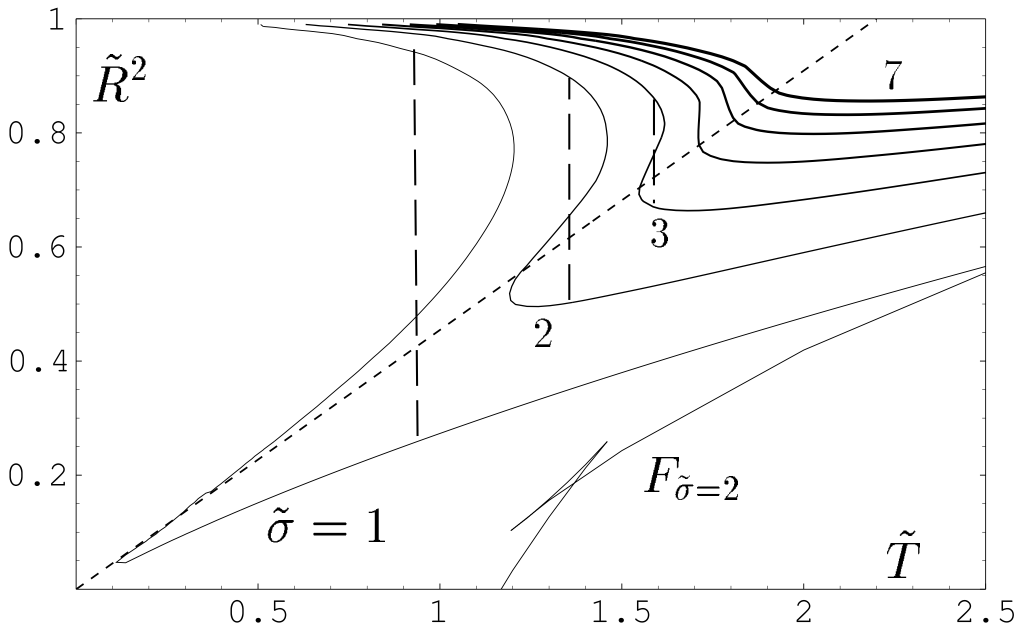
$$H_{\text{eff}} = [H_R + \sum_{i=1}^{N} (R_i^2 f_i - T \log R_i)] \ .$$

Approximation according to Curty and Beck

We compute the partition function by integrating only the phase. For this purpose, we will drop the integration on R_i and search for the minimum of the free energy with respect to R. The minimum of the free energy $F = -k_B T \log Z$ is given through the equation $\delta F / \delta R_i$. Assuming that the gradient of the amplitude is zero, we have

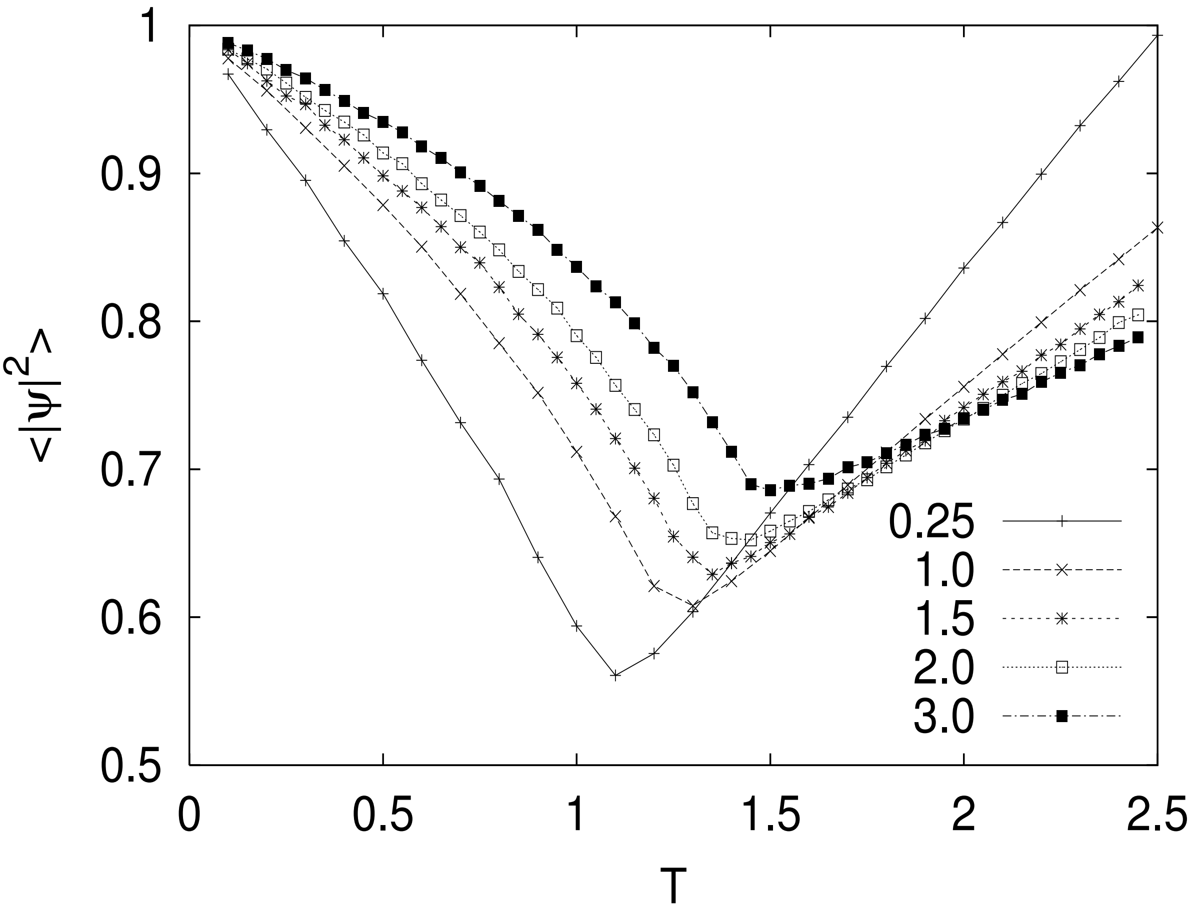
$$\sigma(R^2 + R^4) - \frac{T}{2} + R^2 f(K) = 0.$$

$f(K) = \langle f_i \rangle$ is the expectation value within the XY model of f_i with a dimensionless coupling constant $K = \frac{1}{T} R^2$.



We performed simulations using the single-cluster algorithm to update the direction of the field, and the modulus of ψ is updated with a Metropolis algorithm. We find no first-order phase transition.

Mean square amplitude of the 3D Ginzburg-Landau model on a 15^3 cubic lattice for different values of the parameter σ:



We introduce a generalized Ginzburg-Landau model,

$$H_{\text{eff}} = H - T\kappa \sum_{n=1}^{N} \log R_n \text{ , with } R_n = |\tilde{\psi}_n|.$$

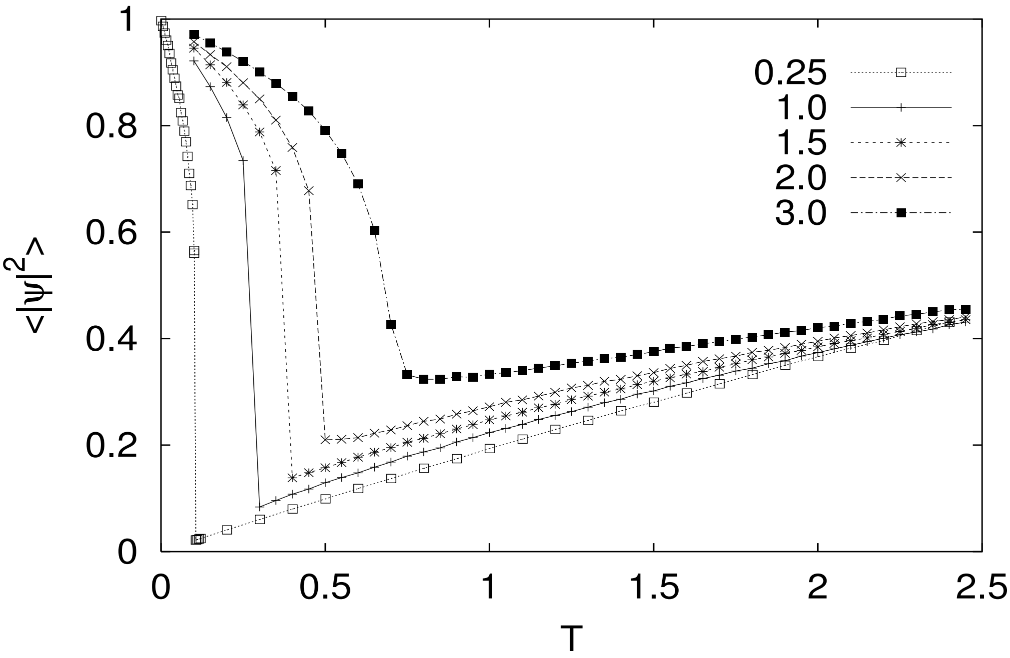
- $\kappa = 1$ corresponds to the Ginzburg-Landau model.

- $-\sum \log R_n$ in H_{eff} tends to suppress field configurations with many nodes $R_n = 0$.

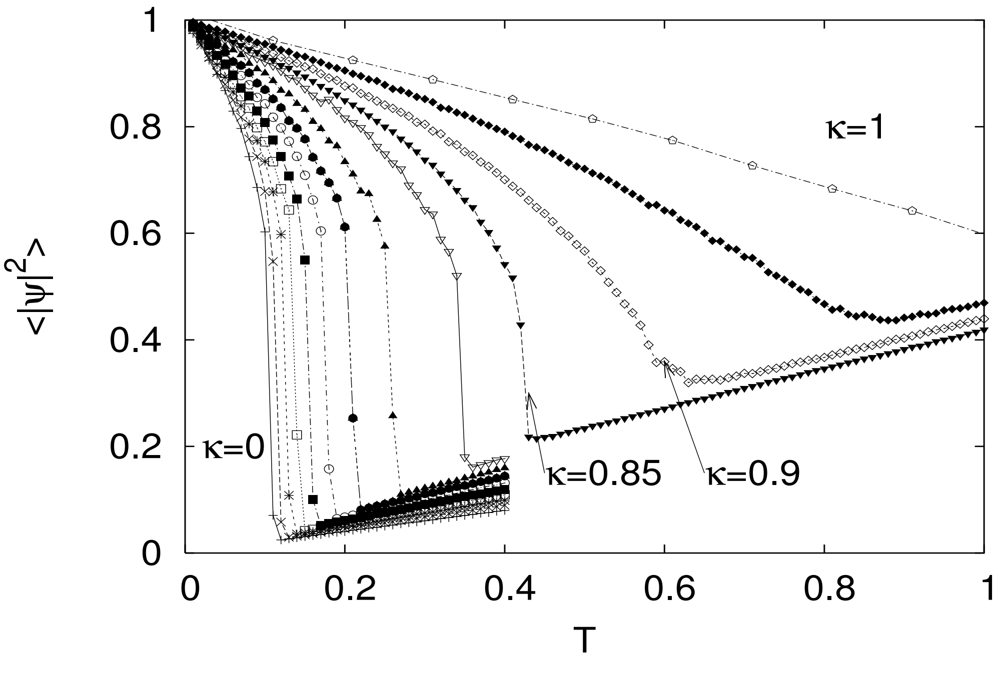
- If this term is omitted, the number of nodes and hence vortices is relatively enhanced.

- In this case a discontinuous, first-order "freezing transition" to a vortex dominated phase can occur.

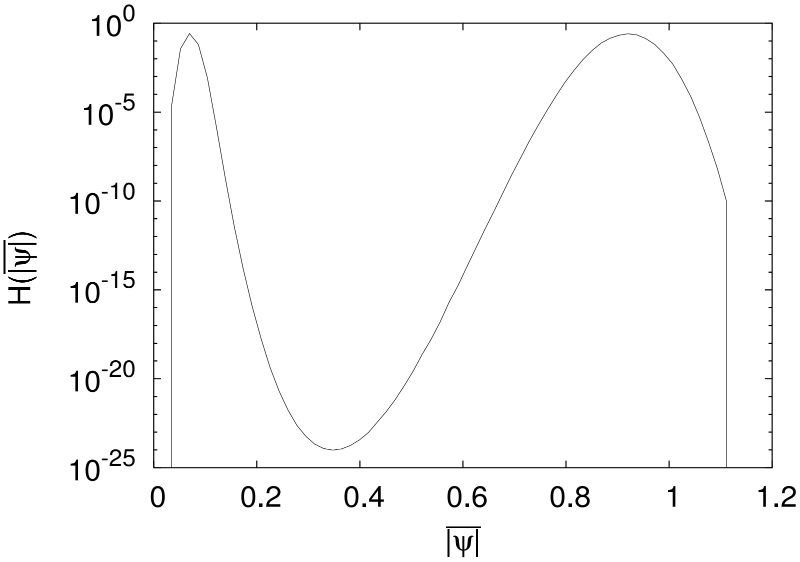
The mean square amplitude $\langle|\psi|^2\rangle$ for different values of the parameter σ with $\kappa = 0$.



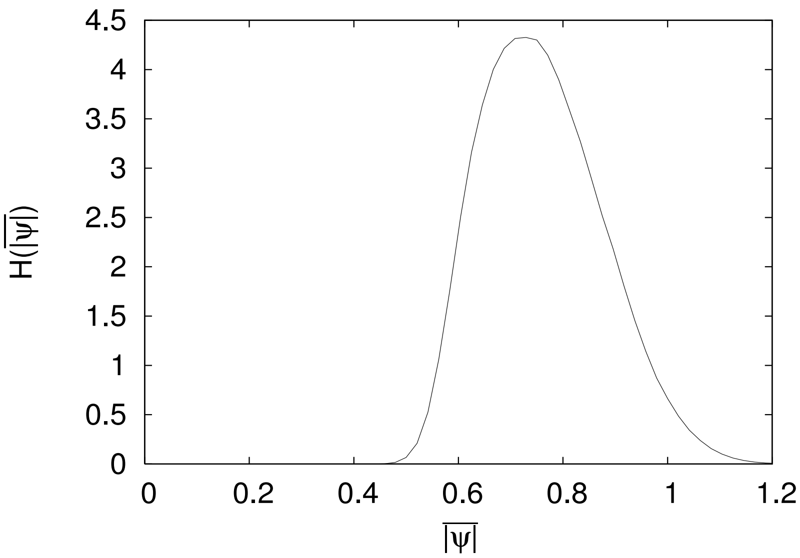
κ dependence of $\langle|\psi|^2\rangle$ for $\sigma = 0.25$.



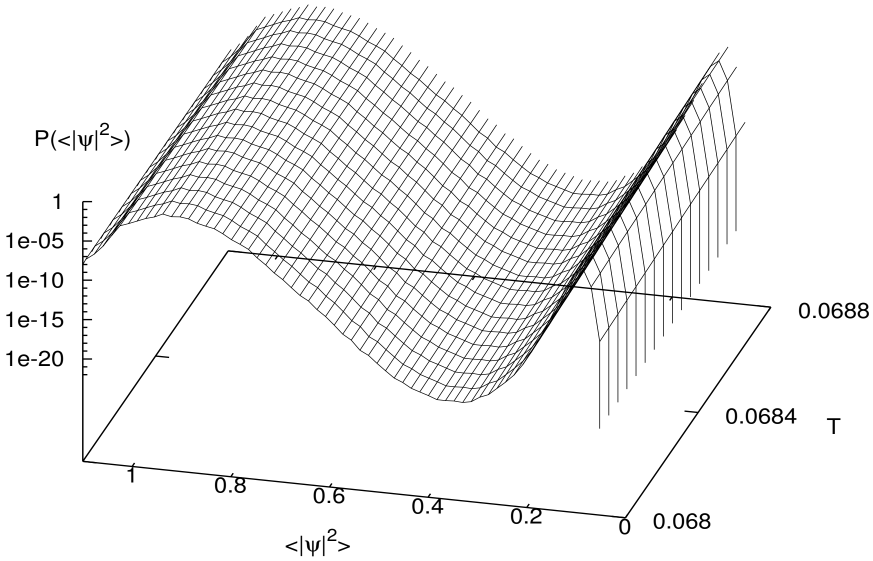
Histogram of the mean modulus $\overline{|\psi|} = \frac{1}{N}\sum_{n=1}^{N}|\psi_n|$ on a logarithmic scale for a 4^3 cubic lattice, $\sigma = 0.25$ and $\kappa = 0$, reweighted to the temperature $T_0 \approx 0.0572$ where the two peaks are of equal height.



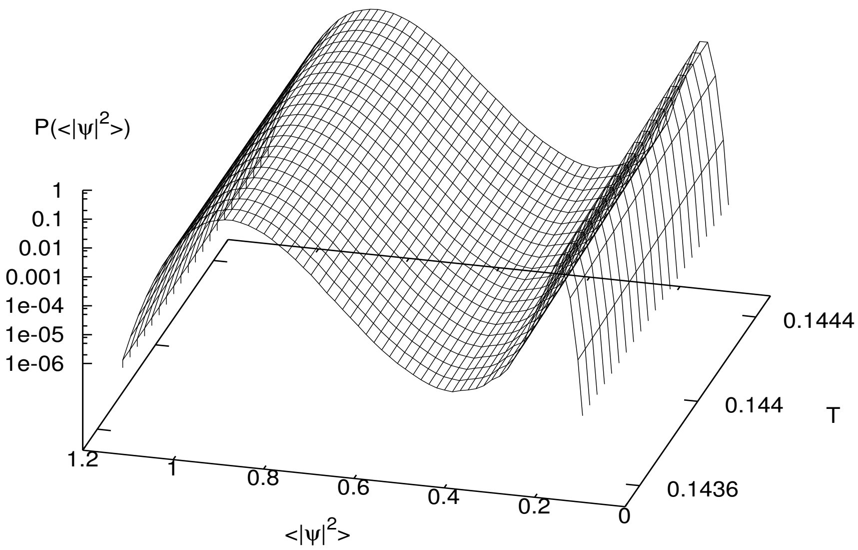
Histogram for the same quantity and lattice size at $T = 1.1$ close to the second-order phase transition for $\sigma = 0.25$ and $\kappa = 1$.



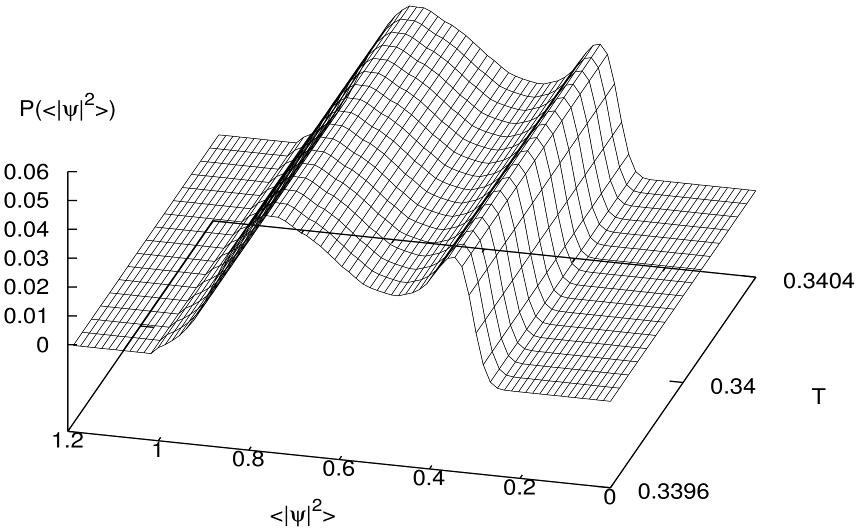
Results of the probability density of $\langle|\psi|^2\rangle$ on a 4^3 cubic lattice for $\sigma = 0.25$ and $\kappa = 0.1$.



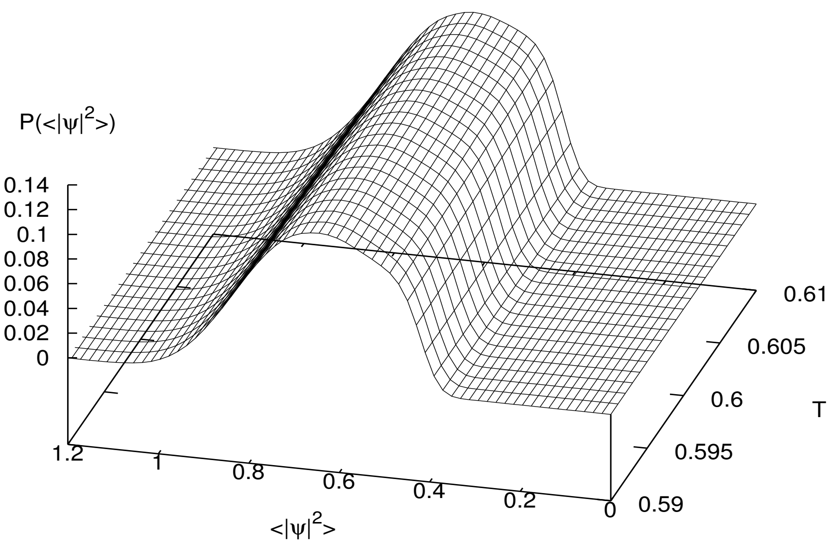
Same result for $\kappa = 0.5$.



Results of the probability density of $\langle|\psi|^2\rangle$ on a 4^3 cubic lattice for $\sigma = 0.25$ and $\kappa = 0.8$.



Same result for $\kappa = 0.9$.



In order to characterize the transition more quantitatively we estimated the interface tension,

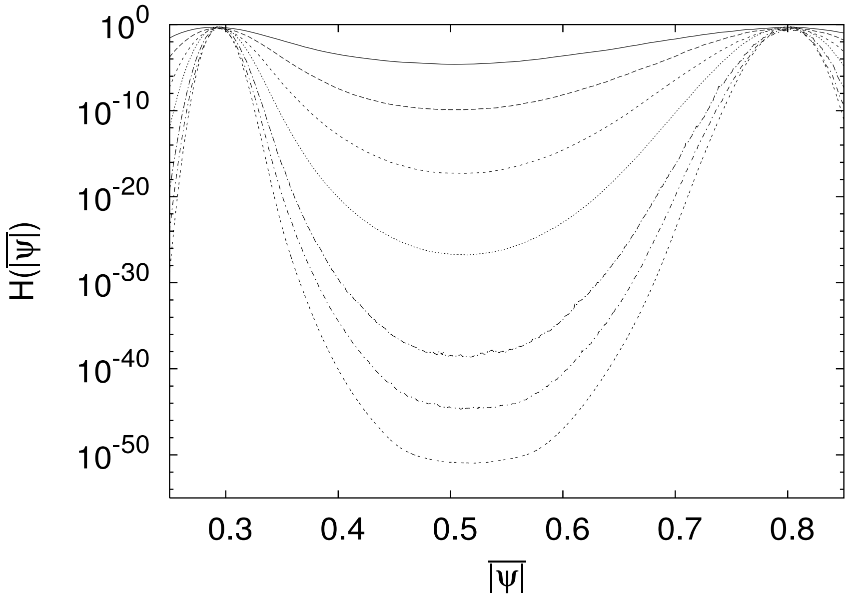
$$F_L^s = \frac{1}{2L^{D-1}} \ln \frac{P_L^{\min}}{P_L^{\max}},$$

where $P_L^{\max}$ is the value of the two peaks and $P_L^{\min}$ denotes the minimum in between. Here it is implicitly assumed that the temperature was chosen such that the two peaks are of equal height which can be achieved by histogram reweighting. For the final estimate of the infinite-volume limit, $F^s = \lim_{L\to\infty} F_L^s$, we performed a fit according to

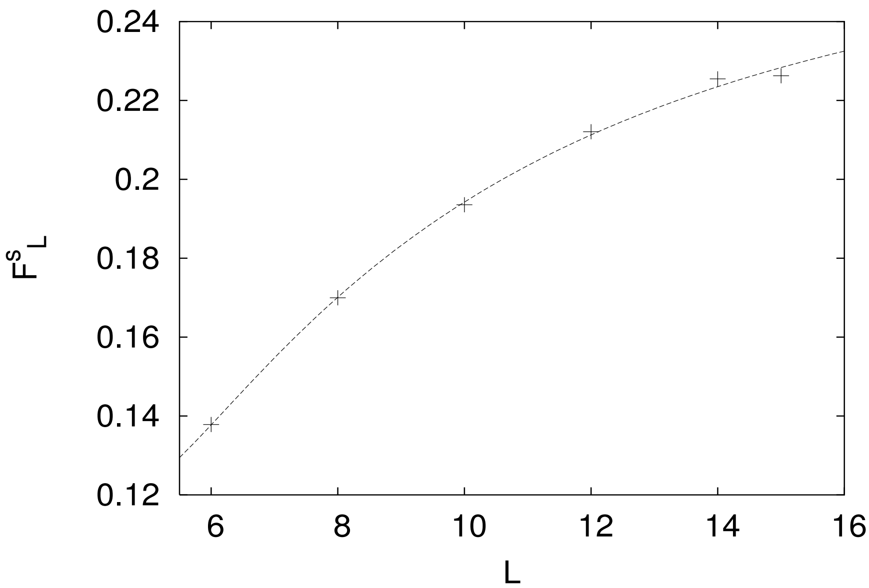
$$F_L^s = F^s + \frac{a}{L^{D-1}} + \frac{b\ln(L)}{L^{D-1}}.$$

The finite-lattice estimates for F_L^s are clearly nonzero, and also the infinite-volume extrapolation yields a pretty large interface tension of $F^s = 0.276(5)$ for $\sigma = 1.5$ and $\kappa = 0$.

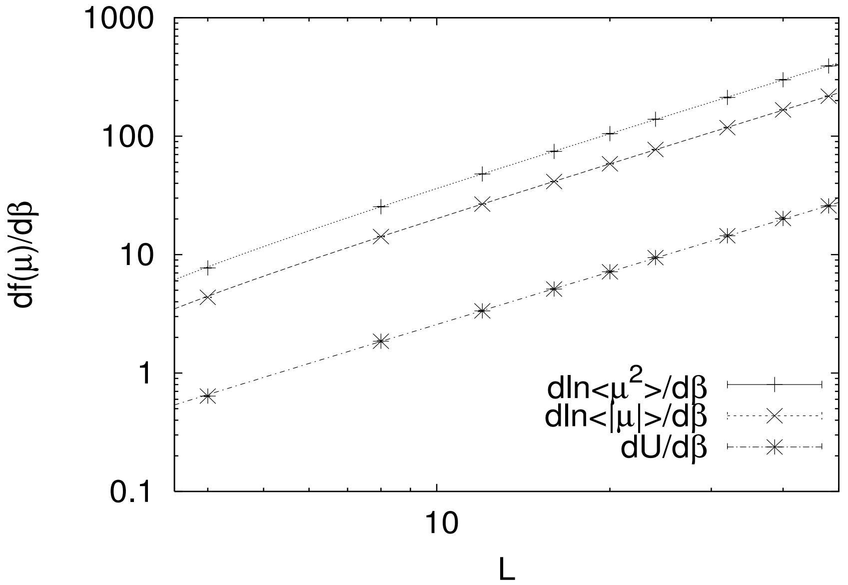
Histogram of the mean modulus $\overline{|\psi|}$ on a logarithmic scale for various lattices, reweighted to temperatures where the two peaks for a given lattice are of equal height.



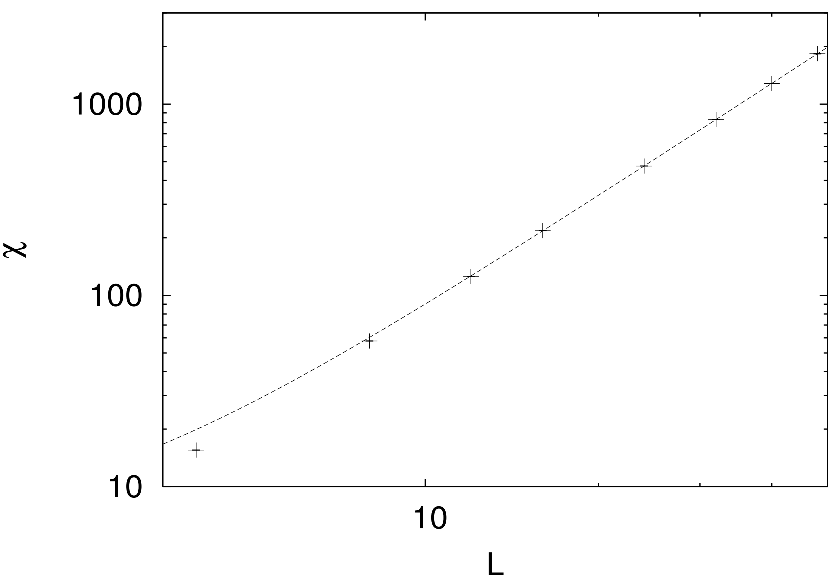
Finite size scaling extrapolation for the interface tension F^s.



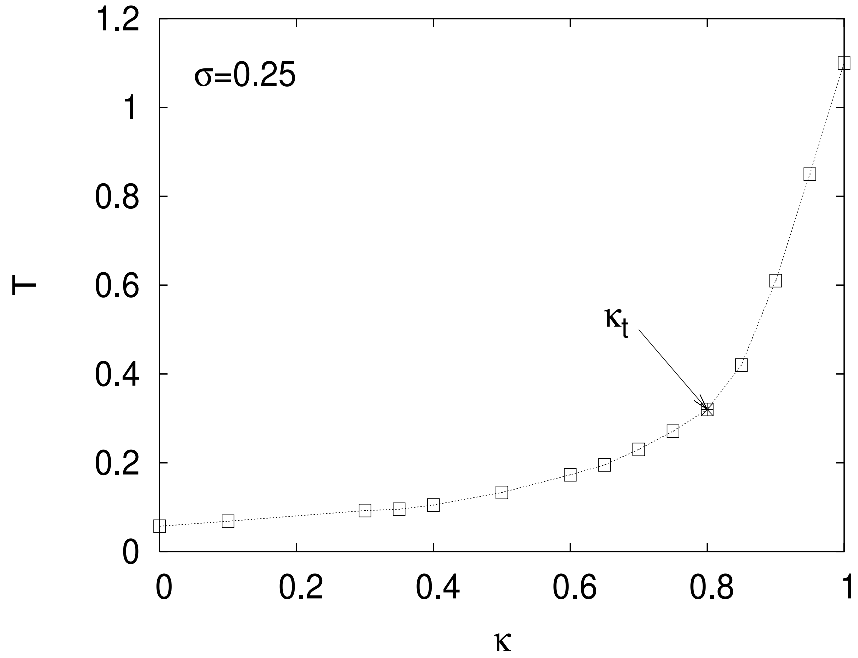
Least-square fits of the FSS ansatz at the maxima locations. The fits using the data from all lattice sizes lead to an overall critical exponent $1/\nu = 1.489(4)$.

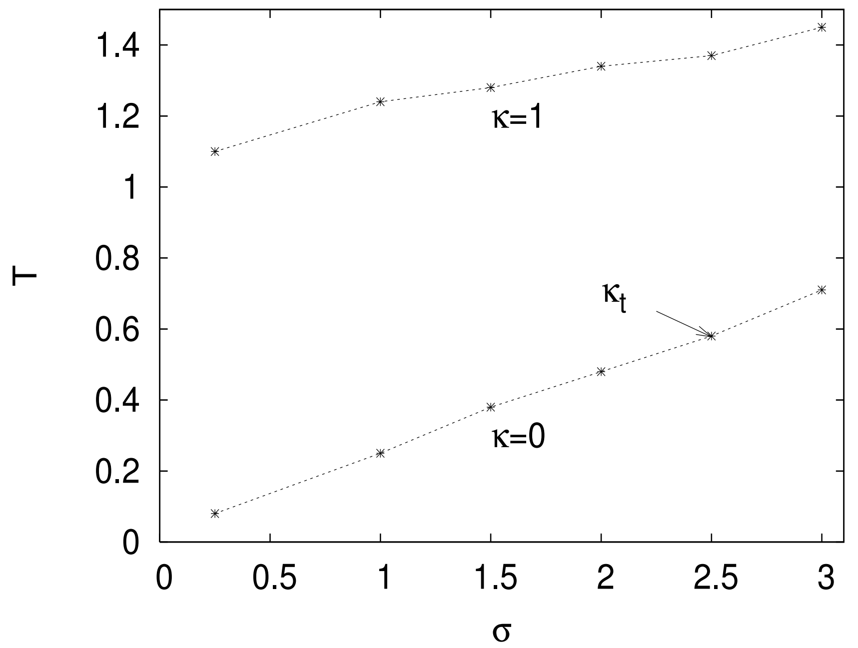


FSS of the susceptibility at β_c. The line shows the three-parameter fit $a + bL^{\gamma/\nu}$, yielding for $L \geq 16$ $\gamma/\nu = 1.944(11)[7]$.



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.





Vortex Condensation in the Generalized $|\psi|^4$ Model

A vortex exists if $m \neq 0$, which is assigned to the object dual to the given plaquette (a site in 2D and a link in 3D).

$$m = \frac{1}{2\pi}([\phi_1 - \phi_2]_{2\pi} + [\phi_2 - \phi_3]_{2\pi} + [\phi_3 - \phi_4]_{2\pi} + [\phi_4 - \phi_1]_{2\pi}) \; ,$$

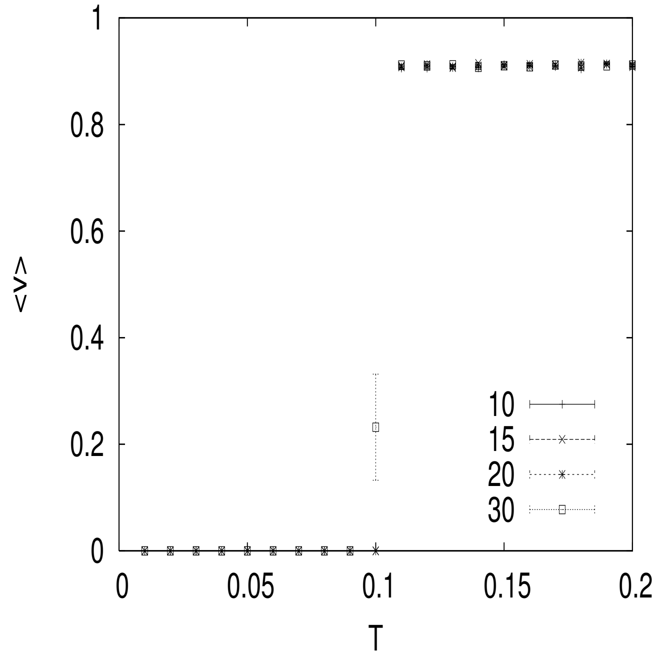
where $[\alpha]_{2\pi}$ stands for α modulo 2π: $[\alpha]_{2\pi} = \alpha + 2\pi n$, with n an integer such that $\alpha + 2\pi n \in (-\pi, \pi]$, hence $m = n_{12} + n_{23} + n_{34} + n_{41}$.

The vortex density v (of vortex points in 2D and vortex lines in 3D):

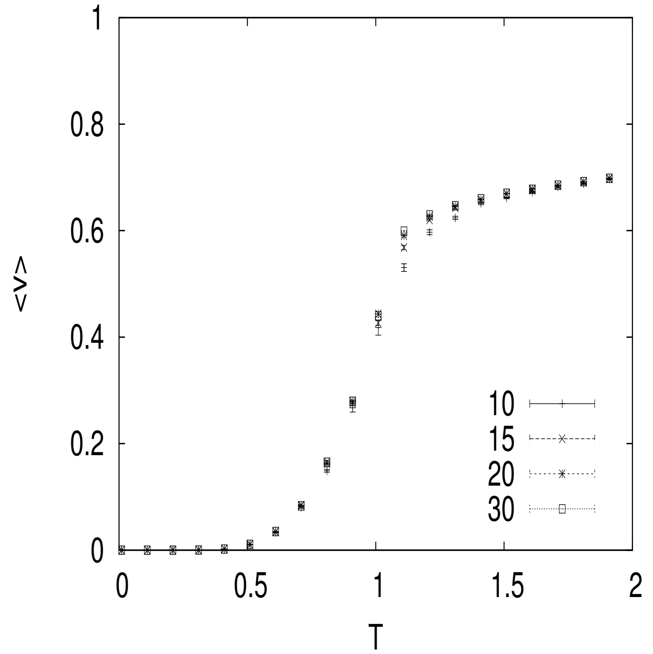
$$v = \frac{1}{L^2} \sum_x |{*m_x}| \quad (2\mathrm{D})$$
$$v = \frac{1}{L^3} \sum_{x,i} |{*l_{i,x}}| \quad (3\mathrm{D})$$

Vortex-line density v on cubic lattices for $\sigma = 0.25$

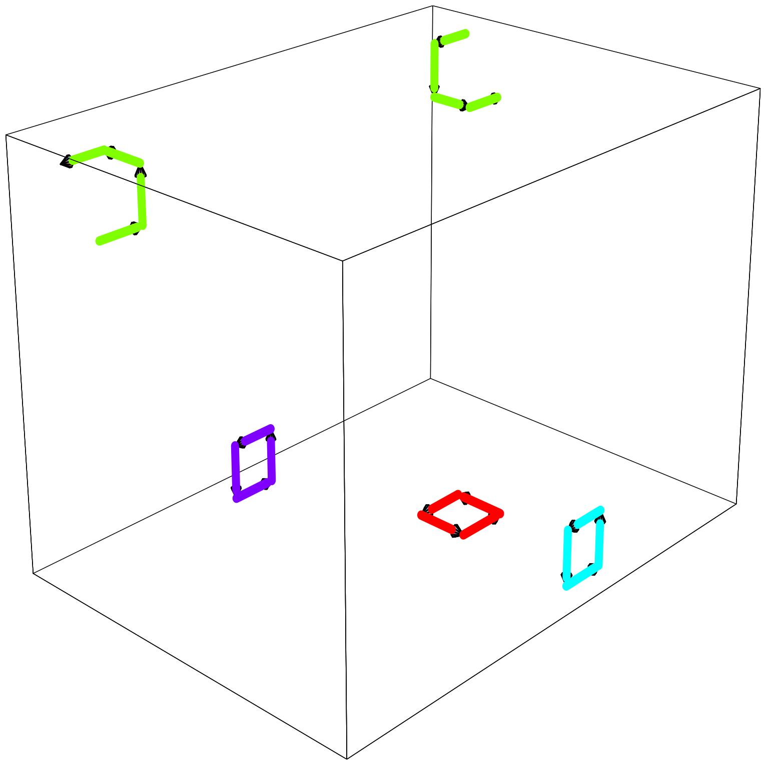
$\kappa = 0$



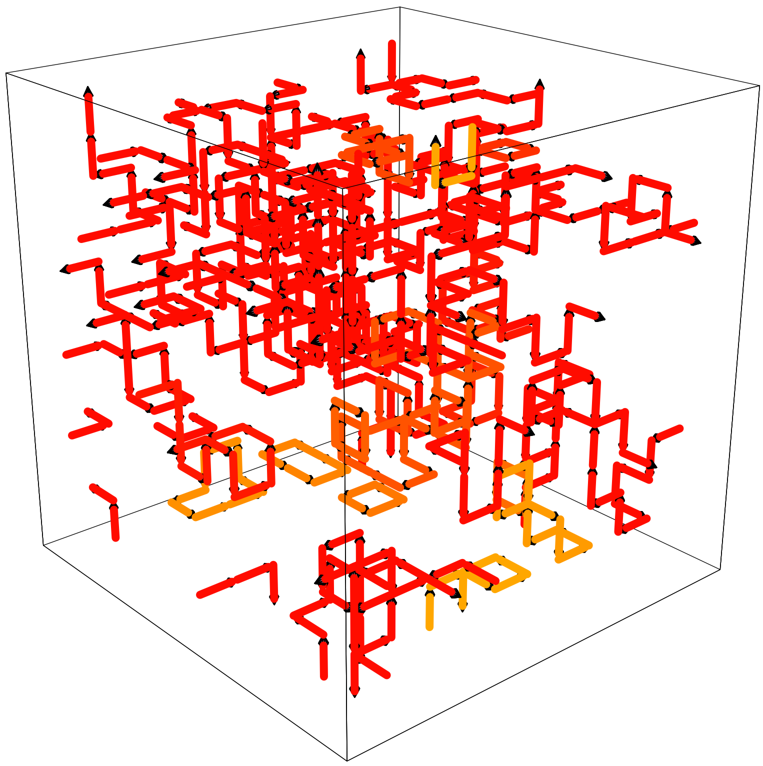
$\kappa = 1$

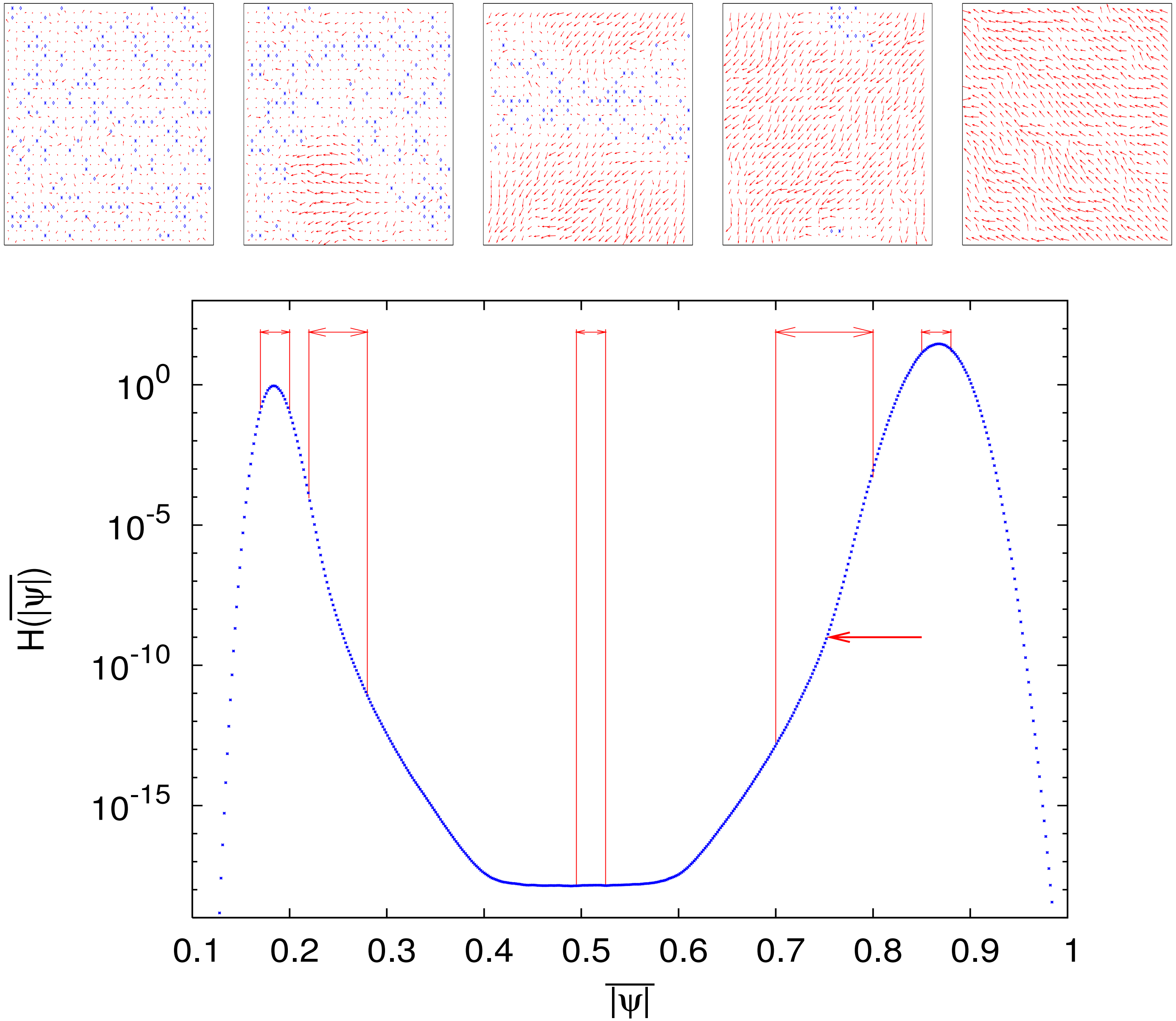


$T = 0.7$



$T = 1.4$





10^{0}
10^{-5}
10^{-10}
10^{-15}
$H(\overline{|\psi|})$
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
$\overline{|\psi|}$

Summary

- The possibility of a phase-fluctuation induced first-order phase transition in the Ginzburg-Landau model as suggested by [1] cannot be confirmed [2].
- Our results suggest that in a modified Ginzburg-Landau model a first-order transition can take place by varying the coefficient κ of the $-\sum \log R_n$ term in the effective Hamiltonian.
- This can be understood by a duality argument as in Ref. [3].
- The vanishing of the dips in the probability densities of $\langle|\psi|^2\rangle$ indicates the tricritical point.
- Our results suggest that the generalized complex $|\psi|^4$ model is a good toy model to study the properties of a vortex proliferation transition.

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

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

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

Next goal

- A study of the tricritical point as a function of σ.
- A study of the properties of vortex proliferation transition.