The Effect of Large Amplitude Fluctuations in the Ginzburg-Landau Phase Transition

G. Alvarez and H. Fort
Instituto de Física, Facultad de Ciencias, Iguá 4225, 11400 Montevideo, Uruguay

The lattice Ginzburg-Landau model in $d=3$ and $d=2$ is a kind of multi purpose or metamodel' which captures the essence of several interesting phenomena of condensed matter: superfluidity, superconductivity and the melting transition. It turns out that in all these phase transitions vortex-like defects (topological singular phase configurations) play a central role condensing above the critical temperature $T_c$ and breaking the ordered state existing below $T_c$.

With the discovery of high-temperature superconductors an entire new area in condensed matter devoted to vortex physics has been opened. A very rich phase diagram for the vortex matter emerged both from the experimental and theoretical side.

The nature of the G-L phase transition in $d=3$ and $d=2$ systems still remains controversial theoretically. For $d=3$, in the early 70’s, Wilson and Fisher showed that the G-L model belongs to the same universality class of the XY model ("phase only" approximation), which is known to exhibit a second-order phase transition. On the other hand, at $T=T_c$ amplitude fluctuations, controlled by the coherence length in units of the lattice spacing $\xi$, are in principle not negligible and they might affect the critical behavior. In that sense, a recent variational approach showed evidences that for $d=3$ the G-L transition can turn first order due to the interplay between phase and amplitude fluctuations when the latter are large enough. For $d=2$ doubt remained if the first order found was not an artifact of the used approximation. However, for $d=2$, we found evidences of a first order transition when amplitude fluctuations are allowed to be large by a suitable choice of the G-L hamiltonian parameters.

In this letter, using a Monte Carlo method we show that: 1) the G-L phase transition becomes first order when $\xi$ is greater than a value $\xi_2 \approx 1$ close to 1, allowing non-negligible amplitude fluctuations and 2) that this change of order is connected with a sudden proliferation of vortices. We worked on square lattices of size $L$ and spacing $a$, we denote the lattice sites by $x$ and the lattice links by $(x, \mu)$ with $\mu = 1, \ldots, d$. We used the parameterization of the Boltzmann exponent $\beta H$ of ref. i.e. in terms of two parameters, the coherence length $\xi$, and a lattice temperature $T_L$, and a dimensionless order parameter $\bar{\psi}$. This parameterization is connected with the ordinary Wilson parametrization $H_W/T$ by:

$$\frac{H_W}{T} = \sum_{x} \sum_{\mu=1}^{d} \frac{1}{2} \left( \psi_{x+\mu} - \psi_{x} \right)^2 + r \left| \psi_{x} \right|^2 + u \left| \psi_{x} \right|^4 = \frac{1}{2T_L} H \sum_{x} \sum_{\mu=1}^{d} \frac{1}{2} \left( \bar{\psi}_{x+\mu} - \bar{\psi}_{x} \right)^2 + \frac{1}{2\xi^2} \left( 1 - \left| \bar{\psi}_{x} \right|^2 \right)^2,$$

(1)

where $\bar{\psi}_{x} = \frac{\bar{\psi}_{x}}{a^{d-2}|r|}$ and $\bar{\psi}_{\infty}$ is the constant value to what $\psi$ approaches infinitely deep in the interior of the superconductor. In what follows we will omit the subscript $L$ of $T$. In the limit of $\xi = 0$ (or $u = \infty$) the radial degree of freedom is frozen and the model reduces to the XY model. The limit we are interested in is just the opposite: $\xi \approx 1$, where large amplitude fluctuations occur.

The calculations were performed using periodic boundary conditions (PBC). As it is common practice, we have discretized the $O(2)$ global symmetry group to a $Z(N)$ to increase the speed of the simulation. For $Z(60)$, we found no appreciable differences when comparing results with previous runs carried out with the full $O(2)$ group in relatively small lattices. We used a sequence of lattice sizes from $L=10$ to $L=64$ for $d=2$ and from $L=6$ to $L=16$ for $d=3$. For the case up to $N \equiv L^d = 508$ sites, we thermalized with usually 20,000-40,000 sweeps and averaged over another 50,000-100,000 sweeps. For greater $N$ larger runs were performed, typically 50,000 sweeps were discarded for equilibration and averaged over 150,000-250,000 sweeps. We
wish to emphasize that for the case $\xi \sim 1$, we are most interested in, no appreciable differences take place by taking $N > 508$ (for instance $8^3$ and $16^3$ give very similar results). The errors for the measured observables are estimated in a standard way by dividing measures in bins large enough to regard them as uncorrelated samples. The following observables were measured to map the phase diagram and analyze the phase transition:

i) The energy density $\varepsilon \equiv \langle H \rangle /N$ and the specific heat $c_V$. $c_V$ was computed both simply as the energy variance per site i.e. $c_V = (\langle H^2 \rangle - \langle H \rangle^2)/N$ and as the temperature derivative of $\varepsilon$. 

ii) The vortex density $v$ (density of loop vortices in $d=3$ and point vortices in $d=2$), which serves as a measure of the phase disorder, defined by:

$$v = \frac{1}{L^2} \sum_{*p} |m_{*p}|,$$

where $*p$ denotes the lattice cell dual to a given lattice plaquette $p$ (a site in $d = 2$ and a link in $d = 3$) and the quantity $m_{*p}$ is the vortex “charge” assigned to $*p$ and measured over the plaquette $p$ as:

$$m_{*p} = \frac{1}{2\pi} (\theta_1 - \theta_2)_{2\pi} + (\theta_2 - \theta_3)_{2\pi} + (\theta_3 - \theta_4)_{2\pi} + (\theta_4 - \theta_1)_{2\pi},$$

where $[\alpha]_{2\pi}$ stands for $\alpha$ modulo $2\pi$. [$\alpha]_{2\pi} = \alpha + 2\pi n$, with $n$ an integer such that $\alpha + 2\pi n \in (-\pi, \pi]$, hence $m_{*p} = n_{12} + n_{23} + n_{34} + n_{41}$ can take three values: 0, ±1 (the value ±2 has a negligible probability).

iii) The helicity modulus $\Gamma_\mu$. $\Gamma_\mu$ measures the phase-stiffness along the direction $\mu$. For a spin system with PBC the helicity modulus measures the cost in free energy of imposing a “twist” equal to $L\delta$ in the phase between two opposite boundaries of the system. $\Gamma_\mu$ is computed using the expression [4]:

$$\Gamma_\mu = \frac{1}{N} \left\{ \langle \sum_x |\bar{\psi}_x| |\bar{\psi}_{x+\mu}| \cos(\theta_{x+\mu} - \theta_x) \rangle - \frac{1}{T} \langle \sum_x |\bar{\psi}_x| |\bar{\psi}_{x+\mu}| \sin(\theta_{x+\mu} - \theta_x) \rangle^2 \right\}. \tag{5}$$

iv) The mean square amplitude $\rho \equiv \langle |\psi|^2 \rangle$ which takes its minimum value at the phase transition.

First, in Fig. 1 we report the phase structure of the model in the $(T, \xi)$ plane for $d=3$ (○) and $d=2$ (●).

For $\xi$ larger than $\xi_{2-1}$ the order of the phase transition changes from continuous (dashed line to first-order (filled line). Specifically, $\xi_{2-1} \simeq 0.8$ ($d=2$) and $\xi_{2-1} \simeq 0.7$ ($d=3$). For $\xi \geq \xi_{2-1}$ $\varepsilon$ exhibits a large hysteresis phenomenon and an histogram with a double peak structure, corresponding to the two coexisting phases, both features characteristic of a first-order transition. In Fig. 2 we present energy histograms for $d=2$ for 2 values of $\xi$: $\xi = 0.85 > \xi_{2-1}$ and $\xi = 0.75 < \xi_{2-1}$, showing the different behavior as $L$ increases: both peaks remain fixed as $L$ increases in the first case while they approach each other as $L$ increases in the second case (besides the peaks are lower and wider). Furthermore, for $\xi = 0.85$ the width of each of the peaks clearly scales as $\sqrt{1/(L^d)} = 1/L$, due to ordinary non-critical fluctuations, while for $\xi = 0.75$ the peaks do not scale this way. (Similar histograms are found for $d=3$ for $\xi \geq \xi_{2-1}$ and $\xi < \xi_{2-1}$).
FIG. 2. Histograms of ε in d=2 for L=10 (below), L=20 (middle) and L=40 (above). (a) ξ=0.85: the two peaks become sharper and their position remain fixed as L increases. (b) Zoom of the right peak showing the scale of its width as 1/L. (c) ξ=0.75: the width of the two peaks do not scales as 1/L and they approach each other as L increases.

Fig. 3 shows the hysteresis phenomenon found when considering heating and cooling runs for d=3 (a completely similar hysteresis diagram is found for d=2 for ξ ≥ ξ_{2→1}).

![Graph](image)

FIG. 3. Hysteresis in d=3, L=14 for ε, ξ = 1 (error bars are smaller than the symbol size).

In order to illustrate the central role played by vortex excitations in triggering and determining the nature of the phase transition, Fig. 4-(a) and 4-(b) show a plot of ρ vs. T for different values of ξ respectively for d=2 and d=3. For coherence lengths larger than ξ_{2→1} we observe a sharp jump in the vortex density v evidencing a sudden proliferation of vortices which coincides with the discontinuity in ε. As long as we decrease ξ the jump becomes more smooth and moves to higher values of Tc. In particular, for d=2, for ξ ≈ 0.1 something very close to the Kosterlitz-Thouless (K-T) behavior is reached. The increase in the density of vortices when amplitude fluctuations are large is due basically to the fact that amplitude fluctuations decrease the energy of vortices enhancing vortex production. The same happens for the XY model with modified interaction \[1\]; in fact, the shape modification of the interaction can be connected with a core energy variation.

![Graph](image)

FIG. 4. Plot of ρ vs. T (error bars are smaller than the symbol size. Left: d=2, L=40; ξ=1 (Δ), ξ=0.8 (∇), ξ = 0.5 (×), ξ = 0.1 (+) and XY (○). Right: d=3, L=12; ξ=1 (Δ), ξ=0.8 (∇), ξ=0.7 (○) and ξ=0.5 (×).

![Graph](image)

FIG. 5. Plot of \( \langle |\psi|^{2} \rangle \) vs. T. (a) d = 2: ξ=2 (□), ξ=1 (Δ), ξ=0.8 (∇), ξ=0.7 (⋆) and ξ=0.5 (×). (b) d = 3: ξ=2 (□), ξ=1 (Δ), ξ=0.8 (∇), ξ=0.7 (⋆) and ξ=0.5 (×).

Figures 5 shows a plot of ρ =\( \langle |\psi|^{2} \rangle \) vs. T for different values of ξ. Note that for ξ > ξ_{2→1} ρ exhibits a sharp drop which coincides with the jump in v and ε (and the drop in \( \Gamma_{\mu} \) not depicted).

Therefore, the nature of the phase transition of the G-L model depends dramatically on the value of the coherence length ξ. For ξ > ξ_{2→1} the transition to a disordered state implies latent heat, a a discontinuous jump of the vortex density and the subsequent abrupt drops in \( \Gamma_{\mu} \) and ρ i.e. all the features of a first order transition. On the other hand, for ξ ≪ 1 the G-L reduces to the XY model (with the more subtle K-T phase transition for d=2). For d=3, the value of ξ_{2→1} ≈ 0.7 is in agreement with ref. \[1\] in which the authors found the ξ^2_{2→1} > 1/4.5 For d=2, the value of ξ_{2→1} ≈ 0.8 belongs to the region (ξ < 1) found in ref. \[2\] such that the RG trajectories cross the first order line of Minnhagen’s \[2\] generic phase diagram for the two-dimensional Coulomb
gas.

To conclude, both for $d=2$ and $d=3$, we offer clear evidences that the order of the phase transition, triggered by vortices, in the G-L model depends on the value of $\xi$ which controls the size of amplitude fluctuations. Whether or not such mechanism based on the interplay between amplitude and phase fluctuations takes place in real systems like high $T_c$ superconductors or in explaining the change in order of the melting transition is something which deserves a more careful analysis.

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