On the Nature of the Phase Transition Triggered by Vortex-Like Deffects in the 2D Ginzburg-Landau Model

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

March 21, 2022

Abstract

The two dimensional lattice Ginzburg-Landau hamiltonian is simulated numerically for different values of the coherence length $\xi$ in units of the lattice spacing $a$, a parameter which controls amplitude fluctuations. The phase diagram on the plane $T - \xi$ is measured. Amplitude fluctuations change dramatically the nature of the phase transition: for values of $\xi/a \simeq 1$, instead of the smooth Kosterlitz-Thouless transition there is a first order transition with a discontinuity in the vortex density $v$ and a sharper drop in the helicity modulus $\Gamma$. Both observables $v$ and $\Gamma$ are analyzed in detail at the crossover region between first and second order which occurs for intermediate values of $\xi/a$.

pacs: 74.20.De, 74.60.-w, 64.60.Cn

1 Introduction

Several condensed matter systems undergo phase transitions which are triggered by vortex-like defects. For instance, this is the case of superfluid helium, superconductors and the melting transition. In particular, the discovery of high-temperature superconductors has boosted the interest in the behavior of vortex lines in the mixed state and opened a new area which regards the physics of vortices as a new state of matter [1]. The Ginzburg-Landau (G-L) model involving a complex field $\psi = |\psi| \exp[i\theta]$ captures the essence of all the above condensed matter systems.

A common assumption when studying vortex-like topological excitations (singular phase $\theta$ configurations) is that amplitude fluctuations can be neglected and that the only relevant degree of freedom is the phase angle $\theta$. The “phase only” approximation is equivalent to consider the limit in which the quartic coefficient of the G-L hamiltonian $u \to \infty$ which freezes the amplitude or equivalently to take the coherence length $\xi = 0$. On the lattice this is the well known XY model. Thanks to the work of Berezinskii [2] and Kosterlitz and Thouless [3] in the early 70’s we have a fair understanding of the XY model in two dimensions. It turns out that a topological phase transition, the so called Kosterlitz-Thouless (KT) transition, takes place driven by the unbinding of vortex-antivortex pairs at a temperature $T_{KT}$. A crucial ingredient of the KT transition is the logarithmic interaction between vortices. For that reason in ref. [3] the authors concluded that in a charged superfluid, due to screening, vortices will always unbind at nonzero temperature. Latter on, it was realized that vortices in sufficiently thin superconducting films indeed interact logarithmically [4]-[5] and it was pointed out that the KT phase transition might also
apply to thin-film superconductors. The 2 dimensional flux line lattice (FLL) melting transition was also regarded as based on a KT-type theory [6]. More recently, it was suggested that some features of the KT theory might be present in under-doped superconducting cuprates [7].

However, the nature of the phase transition triggered by vortices in 2D systems still remains under discussion. By means of Monte Carlo simulations of the XY model with a modified nearest neighbor interaction it was shown that, depending on the value of an additional parameter, continuous as well first-order transitions take place [8]-[10]. The existence of both kinds of phase transitions is in accordance with the richer structure of the 2D Coulomb gas found by Minnhagen and Wallin [11] using self-consistent renormalization group equations and with the tendency towards first-order transition which develops in the case of a strong disorder coupling constant [12]. The 2D FLL also still remains controversial theoretically as well as experimentally. Experimental works and numerical simulations favor a KT-like transition in some cases and a discontinuous one in others [13]. A recent extensive Monte Carlo simulation found a first order transition at a temperature close to the estimated one assuming a KT melting transition [14].

As Bormann and Beck [15] pointed out, at \( T \approx T_c \) the amplitude fluctuations may affect the critical behavior and cannot be neglected. Therefore, instead of the XY model -with fixed amplitude fields- it is worth investigating the effects of vortices when amplitude fluctuations are taken into account. Depending on the chosen parameterization, amplitude fluctuations are controlled by the quartic coefficient \( u \) of the G-L Hamiltonian or by the coherence length \( \xi \). Hence, in this work we simulate the Ginzburg-Landau model (with an amplitude and a phase degree of freedom per point) on a lattice of spacing \( a \) and obtain its two-dimensional phase diagram in the plane \( (T, \xi) \). We will see that the nature of the phase transition of the G-L model diverges dramatically from the KT when the parameter \( u \) is chosen sufficiently small -which in fact is equivalent to take the coherence length \( \xi \approx a \)- and that this is connected with the appearance of a discontinuous jump in the number of vortices.

This article is organized as follows. In section II we define the lattice model, the observables to be computed as well as describe the used Monte Carlo procedure. In section III we report the main numerical results. Section IV is devoted to conclusions and final comments.

2 Description of the model, the observables and the simulation

We will consider square lattices of size \( L \) and spacing \( a \) and denote the lattice sites by \( x \) and the lattice links by \( (x, \mu) \) with \( \mu = 1, 2 \). A straightforward discretization of the continuum Landau-Ginzburg Hamiltonian produces the expression [16]:

\[
\beta H_c = \frac{1}{k_B T} H = \frac{1}{2T_L} a^2 \sum_x \sum_{\mu=1}^{2} \left( \frac{\hbar}{2m} \right)^2 \left( \psi_{x+\alpha \mu} - \psi_x \right)^2 / a^2 + r|\psi_x|^2 + u|\psi_x|^4,
\]

where the superscript \( c \) denotes the ordinary parameterization in the continuum theory, \( \beta = \frac{1}{k_B T} \), \( m \) is the effective mass of the carriers and the coefficients \( r \) and \( u \) are analytic functions of the temperature, with \( u > 0 \) for stability. Instead of working with this parameterization of the Hamiltonian -as we did in ref. [17]- it is better to introduce a dimensionless order parameter: \( \tilde{\psi}_x = \left( \frac{\hbar}{2m} \right)^{3/2} \psi_x \equiv \frac{\psi_x}{|\psi|} \), where \( |\psi| \) is conventionally used because \( \psi \) approaches this value infinitely deep in the interior of the superconductor. Hence the Hamiltonian can be written as

\[
\beta H_c = \frac{1}{k_B T} H = \frac{1}{2T_L} a^2 \sum_x \sum_{\mu=1}^{2} (\tilde{\psi}_{x+\alpha \mu} - \tilde{\psi}_x)^2 / a^2 + \frac{1}{2\xi^2} (1 - |\tilde{\psi}|^2)^2,
\]

where \( \xi \) is the coherence length.
where the lattice temperature $T_L$ and the coherence length $\xi$ are given by

$$
\frac{1}{T_L} = \frac{\hbar^2 |r|}{2muk_B T}, \quad \frac{\xi^2}{a^2} = \frac{\hbar^2}{2m|r|},
$$

in what follows we will denote the lattice temperature simply by $T$, suppressing the subscript $L$. In the limit of $\xi/a = 0$ (or $u = \infty$) the radial degree of freedom is frozen and this model -sometimes said to describe soft spins with non fixed amplitude- becomes the XY model which is said to describe hard spins with fixed amplitude. A more interesting and less well studied limit is just the opposite i.e. $\xi/a \sim 1$ (by (3) small values of the $u$ parameter) which corresponds to large amplitude fluctuations.

We have simulated the Hamiltonian (2) using a Metropolis Monte Carlo standard algorithm. The calculations were performed using periodic boundary conditions (PBC). In order to increase the speed of the simulation we have discretized the $O(2)$ global symmetry group to a $Z(N)$ and compared the results with previous runs carried out with the full $O(2)$ group in relatively small lattices. For the case of $Z(60)$ we found no appreciable differences. Lattices with $L = 10, 20, 24, 32, 40$ and (in some cases) 64 were used. For $L = 10$ and 20 we thermalized with, usually, 20,000-40,000 sweeps and averaged over another 60,000-100,000 sweeps. For $L = 40$ and 64 larger runs were performed, typically 50,000 sweeps were discarded for equilibration and averaged over 200,000 sweeps. We also performed some more extensive runs near $T_c$ for small values of $u$. 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 quantities were measured:

**i) The vortex density $v$.**

The standard procedure to calculate the vorticity on each plaquette is by considering the quantity

$$
m = \frac{1}{2\pi} [\theta_1 - \theta_2]_{2\pi} + [\theta_2 - \theta_3]_{2\pi} + [\theta_3 - \theta_4]_{2\pi} + [\theta_4 - \theta_1]_{2\pi},
$$

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 $m = n_{12} + n_{23} + n_{34} + n_{41}$. If $m \neq 0$, there exists a vortex which is assigned to the object dual to the given plaquette. Hence in the case $d = 2$, $\star m$, the dual of $m$, is assigned to the center of the original plaquette $p$. The vortex “charge” $\star m$ can take three values: 0, ±1 (the value ±2 has a negligible probability). $v$ defined as:

$$
v = \frac{1}{L^2} \sum_x |\star m_x|,
$$

serves as a measure of the vortex density.

**ii) The energy density $\varepsilon = <H>/L^2$ and the specific heat $c_V$.**

Both observables were computed to measure the order of the phase transition. $c_V$ was computed using several procedures: simply as the energy variance per site i.e. $c_V = ( <H^2> - <H>^2 )/L^2$, as the mean of the variance over $B$ bins per site and as the temperature derivative of the energy density $c_V = \lim_{T \to 0} \frac{\Delta\varepsilon}{\Delta T}$.

**iii) The helicity modulus $\Gamma$ [13].**

$\Gamma$ measures the phase-stiffness. 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. $\Gamma$ is obtained in general as a second order derivative of the free energy with respect to $\delta$ -which can be regarded as a uniform statistical vector potential- evaluated for $\delta \to 0$. In such a way one gets the following expression [13], which generalizes the one introduced in ref. [13] to an order parameter with
amplitude as well as phase variations:

\[
\Gamma = \frac{1}{N} \left\{ \left< \sum_{\langle ij \rangle} \right| \psi_i \parallel \psi_j \mid \cos(\theta_i - \theta_j) \right> - \frac{1}{T} \left< \left| \sum_{\langle ij \rangle} \right| \psi_i \parallel \psi_j \mid \sin(\theta_i - \theta_j) \right| \right\}^2\]

(6)

where the primes denote that the sums are carried out over links along one of the 2 directions (x or y).

3 Numerical results

First, in Fig. 1 we report the phase structure of that model in the \((T, \xi)\) plane. The intersection point with the temperature axis \(\xi/a = 0\) corresponds to the XY standard model. Around \(\xi/a \approx 0.8\) the phase transition line, separating the low temperature ordered phase from the high temperature disordered phase, changes from second order to first order. In order to illustrate this change in nature we present histogram results for two temperatures, one above and one below \(T = 0.8\) for sizes \(L = 10, 20, 40\). The double peak structure of the energy histogram corresponding to the 2 coexisting phases, characteristic of a first-order transition, is showed in Fig. 2(a) for \(\xi/a = 0.85\). Both peaks remain fixed as \(L\) increases and the width of each of them clearly scale as \(\sqrt{(<F^2>/T)} = \frac{1}{L}\), due to ordinary non-critical fluctuations, as can be checked from Fig. 2(b). On the other hand, for \(\xi \lesssim 0.75\) the peaks are much lower and wider, they move towards an intermediate value of the energy as \(L\) increases and their width do not scale as \(\frac{1}{L}\) (Fig. 2(c)).

The central role played by vortex excitations in triggering and determining the nature of the phase transition can be seen in Fig. 3-(a) where \(v\) is plotted vs. \(T\) for different values of \(\xi\) and \(L = 20\). For \(\xi/a = 1\) we observe a sharp jump in the vortex density \(v\) (triangles up). As long as we decrease \(\xi\) the jump becomes more smooth and moves to higher values of \(T_c\) until for \(\xi/a = 0.1\) (+ symbols) we get something very close to the KT behavior (circles). The increase in the density of vortices when amplitude fluctuations are large, which is in agreement with the analytical computations of ref. [15], 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 [9], in fact, the shape modification can be straightforwardly connected to a core energy variation. It is interesting to note that when \(\xi \simeq a\) the transition occurs almost from 0 vortex (no bound pairs of vortex-antivortex) to a plasma of vortices. (see Fig. 3-(b)). When measuring \(v\) very close to \(T_c\) from below we found that for \(\xi = 1\), \(n_{pair} \equiv v/2\) becomes 0 except for a very narrow interval -from \(T = 0.115\) to \(T = T_c = 0.12\)- in contrast to what happens in the case of the K-T transition where bound pairs exist for a relatively wide temperature range -from \(T = 0.7\) to \(T = T_c \approx 1\). It is interesting to compare the value of \(v\) for different values of \(\xi\) in all the cases for the same very small reduced temperature \(t = (T_c - T)/T_c \leq 0.01\). We found (for different lattice sizes \(L\)) that \(n_{pair}[\xi/a = 1]\) is one order of magnitude smaller than the \(n_{pair}[\xi/a = 0]\) for the K-T transition; specifically: \(n_{pair}[\xi/a = 1](t = 0.01) \simeq 0.0046\) compared with \(n_{pair}[\xi/a = 0](t = 0.01) \simeq 0.05\).

The scarcity of bound pairs of vortex-antivortex below \(T_c\) for the large fluctuations regime \((\xi \sim a)\) can be explained in terms of the behavior of their free energy \(F_{pair} = E_{pair} - TS_{pair}\) at \(T \sim T_c\) from below. Roughly, \(E_{pair} \simeq 2E_c\), where \(E_c\) is the vortex core energy, and \(S_{pair} \sim \ln(\xi/a)\). The three quantities \(S_{pair}, E_c, T_c\) all decrease as \(\xi\) increases making difficult to disentangle the “energetic” contribution to \(v\), proportional to \(\exp[-E_{pair}/T]\), from the “entropic” contribution \(\sim 1/\xi^2\). Fig. 4 shows a plot of \(v\) vs. \(\xi\) always measured at the corresponding reduced temperature \(t = 0.01\) and fittings with the energetic and entropic behaviors. For the intermediate range of \(\xi\), although it is not easy to predict the behavior of the energetic factor, the entropy seems to be the main responsible for lowering the density of bound pairs. From \(\xi/a \sim 1\), \(T_c\) starts to decrease with \(\lambda\) faster than \(E_{pair}\) and thus \(\exp[-F_{pair}/T]\) decreases more and more sharply making smaller and smaller the probability of bound pairs of vortex-antivortex.
Figure 1: Phase diagram in the $(T, \xi/a)$ plane for $L = 40$. The phase transition from the ordered phase to the disordered phase changes from second order (dashed line) to first order (filled line) at $\xi/a \simeq 0.8$.

Figure 2: Histograms of $\epsilon$ for $L = 10$ (below), $L = 20$ (middle) and $L = 40$ (above). (a) $\xi/a = 0.85$: the 2 peaks become sharper and their position remain fixed as $L$ increases. (b) Zoom of the right peak showing that its width scales as $1/L$. (c) $\xi/a = 0.75$: the width of the 2 peaks do not scale as $1/L$ and they approach each other as $L$ increases.
Figure 3: (a) $v$ vs. $T$ for $\xi/a = 1$ (triangles up), $\xi/a = 0.8$ (triangles down), $\xi/a = 0.5$ (×), $\xi = 0.1$ (+), and the XY model (circles). (b) Zoom of (a) showing the discontinuity of $v$ at $T_c$ when $\xi/a = 1$.

Figure 4: $v$ vs $\xi/a$ (asterisks with error bars) measured on a $20 \times 20$ lattice always at the reduced temperature $t = 0.01$ for that value of $\xi/a$. “entropic fitting” $\sim 1/\xi^2$ (circles) and “energetic fitting” $\sim \exp[-E_{\text{pair}}/T_c]$ (solid line).
Figure 5: $\varepsilon$, $v$ and $\Gamma$ for $\xi/a = 1$ for sizes: $L = 10$ (circles), $L = 20$ (diamonds) and $L = 40$ (squares). Error bars for $\varepsilon$ and $v$ are smaller than the symbol sizes.

Figure 6: $\varepsilon$, $v$ and $\Gamma$ for $\xi/a = 0.5$ for sizes: $L = 10$ (circles), $L = 20$ (diamonds) and $L = 40$ (squares). Error bars for $\varepsilon$ and $v$ are smaller than the symbol sizes.
Figures 5–7 show plots of $\varepsilon$, $v$ and $\Gamma$ for $\xi/a = 1, 0.5$ and 0.1. For $\xi/a = 1$ the transition is clearly first-order: we observe latent heat and discontinuous changes in $v$ and $\Gamma$ at $T = T_c$. On the other hand, for $\xi/a = 0.1$ the results are similar to those of the KT transition. In particular, the energy is very close to the XY energy.

4 Conclusions

Therefore, in the G-L model the nature of the phase transition depends on the value of the coherence length parameter $\xi/a$ (which controls the thermal fluctuations of vortex cores) and the following picture emerges:

1) For $\frac{\xi}{a} > 0.8$ the density of vortices experiments a discontinuous jump which coincides with a first order transition with large latent heat and a sharp jump in $\Gamma$ all at a $T_c$ which decreases with $\xi$. This is the LGW-regime in which a sudden proliferation of vortices takes place instead of the unbinding of the much more smooth KT-regime.

2) For $\frac{\xi}{a} \ll 1$ we get basically the XY model ($|\psi| = 1$) and the more subtle KT transition (with an unobservable essential singularity in the specific heat at $T_c$ and a much more small non-universal maximum above $T_c$ and a universal jump in $\Gamma$). The number of vortices and the energy evolve smoothly across the transition.

3) For intermediate values of $\xi$ we have an interpolating regime between LGW and KT.

Whether or not a large enough increment of $\frac{\xi}{a}$ or $u$ to alter the nature of the phase transition driven by vortices can be accomplished by varying some thermodynamic parameter, for instance the pressure, is something which deserves investigation.

This change in the nature of the phase transition when amplitude fluctuations of $\psi$ are non negligible
\( (\xi/a \sim 1) \) is in agreement with very recent variational computations for the same model \([20]\). Furthermore, we found first order transitions for \( \xi/a > 0.8 \), an interval which is included into the less restrictive of ref. \([5]\) in which for \( \xi/a > 0.5 \) the authors found that the RG trajectories cross the first order line of Minnhaegen’s generic phase diagram for the two-dimensional Coulomb gas.

Finally, our analysis could shed light on the nature of the melting transition. It is possible that the order of the melting transition in 2D depends on the particular conditions and details of the studied specimen which in turn translate into considerable different values of the coherence length \( \xi/a \).

Work supported in part by CSIC, Project No. 052 and PEDECIBA.

References

[1] G. Blatter, M.V. Feigelman, V.B. Geshkenbein, A.I. Larkin and D. Vinokur, Rev. Mod. Phys. 66, 1125 (1994) and references therein.
[2] V.L. Berezinskii, Sov. Phys. JETP 34, 610 (1972).
[3] J.M. Kosterlitz and D.J. Thouless, J. Phys. C6, 1181 (1973)
[4] M. R. Beasley, J.E. Mooij and T.P. Orlando, Phys. Rev. Lett. 42, 1165 (1979).
[5] A.F. Hebard and A.T. Fiory, Phys. Rev. Lett. 50, 1603 (1983).
[6] S. Doniach and B.A. Huberman, Phys. Rev. Lett. 42, 1169 (1979).
[7] J. Corson, R. Mallozzi, J. Orenstein, J.N. Eckstein and I. Bozovic, Nature 398, 221 (1999).
[8] A. Jonsson, P. Minnhagen and M. Nylen, Phys. Rev. Lett. 70, 1327 (1993).
[9] E. Domany, M. Schick and R. Swendsen, Phys. Rev. Lett. 52, 1355 (1984).
[10] J. E. van Himbergen, Phys. Rev. Lett. 53, 5 (1984).
[11] P. Minnagen and M. Wallin, Phys. Rev. B36, 5620 (1987).
[12] S. E. Korshunov, Phys. Rev. B46, 6615 (1992).
[13] K.J. Strandburg, Rev. Mod. Phys. 60, 161 (1988).
[14] Y. Kato and N. Nagaosa, Phys. Rev. B47, 2932 (1993).
[15] D. Bormann and H. Beck, Jour. Stat. Phys. 76, 361 (1994).
[16] M. N. Barber, Phys. Rep. 59, 375 (1980).
[17] G. Alvarez and H. Fort, cond-mat/0006341. In this letter we considered the usual parameterization in lattice quantum field theory for the Euclidean action.
[18] M.E. Fisher, M.N. Barber and D. Jasnow, Phys. Rev. A8, 1111 (1973).
[19] An analogous expression for the case of a granular superconductor appears in C. Ebner and D. Stroud, Phys. Rev. B28, 5053 (1983). In a similar way is calculated the orbital magnetic susceptibility, see for instance: A. Sewer, H. Beck, X. Zotos; Physica C 317-318, 475 (1999).
[20] H. Beck and P. Curty private communication.
[21] Ch. Leeman et al, Phys. Rev. Lett. 64, 3082 (1990).