Phase Transitions Driven by Vortices in 2D Superfluids and Superconductors: From Kosterlitz-Thouless to 1st Order

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The Landau-Ginzburg-Wilson hamiltonian is studied for different values of the parameter $\lambda$ which multiplies the quartic term (it turns out that this is equivalent to consider different values of the coherence length $\xi$ in units of the lattice spacing $a$). It is observed that amplitude fluctuations can change dramatically the nature of the phase transition: for small values of $\lambda$ ($\xi/a > 0.7$), instead of the smooth Kosterlitz-Thouless transition there is a first order transition with a discontinuous jump in the vortex density $v$ and a larger non-universal drop in the helicity modulus. In particular, for $\lambda$ sufficiently small ($\xi/a \geq 1$), the density of bound pairs of vortex-antivortex below $T_c$ is so low that, $v$ drops to zero almost for all temperature $T < T_c$.

Vortices play a central role in explaining the phase diagram and properties of superfluid systems both neutral and charged. The discovery of high-temperature superconductors has boosted the interest in the dynamics of the vortex lines in the mixed state and opened a new area which regards the physics of vortices as a new state of matter [4].

Superfluid films and Josephson junction arrays in two dimensions are often described by XY-type models in which the unique microscopic degrees of freedom are phases. Thanks to the work of Berezinskii [2] and Kosterlitz and Thouless [3] in the early 70’s we have a fair understanding of the standard XY model in two dimensions. In their theory a thermodynamic phase transition, the Kosterlitz-Thouless (KT) transition is driven by the unbinding vortices (singular phase configurations) at a temperature $T_{KT}$. In refs. [4]-[6] it was pointed out that the KT phase transition might also apply to thin-film superconductors and some experimental evidence was discussed. In particular, the analysis of the 2 dimensional flux line lattice (FLL) melting transition of ref. [5] is based on a KT-type theory. 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 driven by vortices in 2D 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].

Our approach to the nature of the phase transition driven by vortices in 2D still remains under discussion. By noting that right at the (expected vortex-pair unbinding) transition the amplitude fluctuations cannot be considered as weak anymore and thus may affect the critical behavior [13]. Therefore, instead of the XY model -with fixed amplitude fields- it is worth investigating the effects of vortices when amplitude fluctuations are not neglected. Hence, in this letter we analyze the more general Landau-Ginzburg-Wilson (LGW) [14] lattice Hamiltonian, in terms of a complex field $\psi = |\psi| \exp i \theta$ ($|\psi| \neq \text{constant}$) and two parameters $K$ and $\lambda$ [15]:

$$\beta H = -2K \sum_{x} \sum_{\mu} |\psi_{x}| |\psi_{x+\alpha \mu}| \cos(\theta_{x+\alpha \mu} - \theta_{x}) + \sum_{x} [\lambda(|\psi_{x}|^2 - 1)^2 + |\psi_{x}|^2], \quad (1)$$

where $\beta = 1/T$, $a$ is the lattice spacing, $x$ denotes the lattice sites and the index $\mu = 1, 2$. We will
show that the nature of the phase transition of this model diverges dramatically from the KT when the parameter $\lambda$ 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 sharp jump in the number of vortices.

A straightforward discretization of the continuum Landau-Ginzburg Hamiltonian produces the expression $^{[4]}$

$$
\beta H = \beta a^2 \sum_x \sum_{\mu=1}^{2} \frac{\hbar^2}{2m} (\psi^c_{x+a\mu} - \psi^c_x)^2 / a^2 + r|\psi^c_x|^2 + u|\psi^c_x|^4,
$$

(2)

where the superscript $c$ in $\psi$ denotes the ordinary parameterization in the continuum theory, $m$ is the effective mass of the carriers and the coefficients $r$ and $u$ are analytic functions of the temperature, with $u > 0$ for stability. Introducing a dimensionless order parameter: $\bar{\psi}_x = (\frac{2a}{\pi})^{\frac{1}{4}} \psi^c_x$ and writing

$$
\beta H = \frac{1}{k_BT} a^2 \sum_x \sum_{\mu=1}^{2} (\bar{\psi}_{x+a\mu} - \bar{\psi}_x)^2 / a^2 + \frac{1}{2\xi^2} (1 - |\bar{\psi}_x|^2)^2,
$$

(3)

where $\frac{1}{k_BT} = \frac{\hbar^2}{2ma} \beta$ and $\xi$ is the coherence length given by $\xi^2 = \frac{\hbar^2}{2m|\lambda|}$. Parameterizations (1) and (3) are connected by the relations:

$$
\frac{\xi}{a} = \left( \frac{K}{1 - 2\lambda - 4K} \right)^{\frac{1}{4}}, \quad T = \frac{\lambda(\xi/a)^2}{K^2} = \frac{\lambda}{K|4K + 2\lambda - 1|}.
$$

(4)

In the limit of $\lambda = \infty$ 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. small values of the $\lambda$ parameter. By $^{[3]}$ small values of $\lambda$ correspond to a large $\xi$ in units of $a$ i.e. $\lambda$ and $1/\xi^2$ are the self-interaction coefficients respectively in $^{[1]}$ and $^{[2]}$ regulating amplitude fluctuations.

We have simulated the Hamiltonian $^{[4]}$ using a Monte Carlo algorithm. The calculations were performed on square $L \times L$ lattices with 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 $L = 10, 20, 24$ we thermalized with, usually, 20,000-40,000 sweeps and averaged over another 60,000-100,000 sweeps. For $L = 32, 40$ 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 $K_c$ for small values of $\lambda$. 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

$$
m = \frac{1}{2\pi} (|\theta_1 - \theta_2|_{2\pi} + |\theta_2 - \theta_3|_{2\pi} + |\theta_3 - \theta_4|_{2\pi} + |\theta_4 - \theta_1|_{2\pi}),
$$

(5)

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 $d = 2$, $*m$, the dual of $m$, is assigned to the center of the original plaquette $p$. The vortex “charge” $*m$ can take three values: 0, ±1 (the value ±2 has a negligible probability). $v$ defined as:

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

(6)
serves as a measure of the vortex density. ii) The energy density $\varepsilon = <H>/L^2$ and the specific heat $C_v$, which were computed to measure the order of the phase transition. iii) The helicity modulus $\Gamma$ which 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 [17], which generalizes the one introduced in ref. [16], to an order parameter with amplitude as well as phase variations:

$$\Gamma = \frac{1}{N} \left\{ <\sum_{<ij>} \left| \psi_i \right| \left| \psi_j \right| \cos(\theta_i - \theta_j) > -k <\sum_{<ij>} \left| \psi_i \right| \left| \psi_j \right| \sin(\theta_i - \theta_j) > \right\}, \quad (7)$$

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

Fig. 1-(a) shows a plot of $v$ vs. $T$ for different values of $\lambda$ and $L = 40$. For $\lambda = 0.01 (\xi \cong 0.94$ we observe a sharp jump in the vortex density $v$ (triangles up). As long as we increase $\lambda$ the jump becomes more smooth and moves to higher values of $T_c$ until for $\lambda = 10 (+$ symbols) we get something very close to the $\lambda \to \infty$ KT behavior (circles). The increase in the density of vortices when amplitude fluctuations
are large is in agreement with the analytical computations of ref. [13]. What is new is the fact that, when \( \xi \simeq a \) (\( \lambda \approx 0.01 \)), the transition occurs almost directly from 0 vortex to a plasma of vortices i.e. the bound pairs of vortex-antivortex seem to play no major role. Fig. 1-(b) is a zoom of 1-(a) showing the difference between \( \lambda = 0.01 \) and \( \lambda = 0.1 \) below \( T_c \): for \( \lambda = 0.1 \) \( v \) drops to non-zero values due to the existence of vortex-antivortex pairs while for \( \lambda = 0.01 \) \( v \) drops much more sharply to 0 signaling the sudden extinction of vortices.

The different behavior of \( v \) above \( T_c \) between the large fluctuating amplitude LGW-regime \( \frac{\xi}{a} \sim 1 \) and the KT-regime \( \frac{\xi}{a} \ll 1 \) is because amplitude fluctuations -governed by the \( \lambda \) parameter- indeed decrease the energy of vortices enhancing vortex production. The same happens for the XY model with modified interaction \[10\]; in fact, the shape modification can be straightforwardly connected to a core energy variation.

The scarcity of bound pairs of vortex-antivortex below \( T_c \) for the extreme fluctuations regime (very small values of \( \lambda \) or \( \xi \sim a \)) 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, \( E_{pair} \sim 2E_c \), where \( E_c \) is the vortex core energy, and \( S_{pair} \sim \ln(\frac{L^2}{\xi^2}) \). The three quantities \( S_{pair}, E_c \) and \( T_c \) all decrease as \( \lambda \) decreases making difficult to disentangle the "energetic" contribution to \( v \), proportional to \( \exp[-E_{pair}/T_c] \), from the "entropic" contribution \( \sim 1/\xi^2 \). For the intermediate range of \( \lambda \) (or \( \xi \)), 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 \[18\]. From a \( \lambda \) sufficiently small, \( T_c \) 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.

Figures 2-4 show plots of \( \varepsilon, v \) and \( \Gamma \) for \( \lambda = 0.01, 0.1 \) and 10. For \( \lambda = 0.01 \) 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 \( \lambda = 10 \) (or \( \frac{\xi}{a} \simeq \frac{1}{\sqrt{42}} \)) the results are similar to those of the XY model. In particular, we get something close to the KT universal jump \( \Delta \Gamma \sim \frac{2}{\xi^2} \). As long as \( \lambda \) decreases we get a larger non universal jump in \( \Gamma \). \( \lambda = 0.1 \) corresponds to something in between first order and KT.
FIG. 2. $\varepsilon$, $v$ and $\Gamma$ vs. $T$, $\lambda = 0.01$ for sizes: $L = 10$ (circles), $L = 20$ (diamonds) and $L = 40$ (squares). Error bars for $\varepsilon$ and $v$ are smaller than the symbol sizes.

FIG. 3. $\varepsilon$, $v$ and $\Gamma$ vs. $T$, $\lambda = 0.1$ for sizes: $L = 10$ (circles), $L = 20$ (diamonds) and $L = 40$ (squares). Error bars for $\varepsilon$ and $v$ are smaller than the symbol sizes.
The double peak structure corresponding to the 2 coexisting phases, characteristic of a first-order transition, is showed in Fig. 5(a) for \( \lambda = 0.01 \) and sizes \( L = 10, 20 \) and 40. The width \( w \) of each of the peaks clearly scale as \( w \sim \sqrt{\frac{T_c}{T}} = \frac{1}{L} \) due to ordinary non-critical fluctuations. Fig 5(b) is a zoom of the right peak centered around the higher energy phase. It shows that \( w \sim 0.1(L = 40), w \sim 0.2(L = 20) \) and \( w \sim 0.4(L = 10) \).

Therefore, one has a simple model in which the nature of the phase transition depends on the value of one parameter (\( \lambda \) or \( \xi/a \)) which controls the thermal fluctuations of vortex cores and from which the following picture emerges:

1. For \( \lambda < 0.1 \) or \( \frac{T_c}{T} \sim 1 \) the density of vortices experiments an abrupt jump which coincides with a first order transition with large latent heat and a non universal jump in \( \Gamma \) all at a \( T_c \) which grows with \( \lambda \). This is the LGW-regime as opposed to the much more smooth KT-regime. In particular, for sufficiently small values of \( \lambda \) (for instance \( \lambda = 0.01 \)) below \( T_c \) \( v \) drops to zero i.e. the number of measured bound pairs of vortex-antivortex is negligible compared with the number found in the KT transition.

2. For \( \lambda \geq 10 \) or \( \frac{T_c}{T} \ll 1 \) we get basically the XY model (\( |\psi| \) is fixed = 1 for all \( K \)) 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 \( \lambda \) (0.1 \( \leq \lambda < 10 \)) we have an interpolating regime between LGW and KT.
Whether or not a large enough increment of $\xi/a$ or $\lambda$ 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 not negligible ($\lambda \leq 0.1$) is in agreement with very recent variational computations for the same model [19]. Furthermore, we checked that all the couples of values $(K_c, \lambda)$ for what we found a first order transition are such that equation (4) gives $0.7 < \xi/a < 1.1$ in complete accordance with figure 6 of ref. [13] from which we can see that for $\xi/a$ bigger than 0.5 the RG trajectories cross the first order line of Minnhaen’s [11] generic phase diagram for the two-dimensional Coulomb gas [20]. The jump in $\Gamma$ larger than the universal value seems consistent with experiments on thin films HTc superconductors [21].

Finally, our analysis could shed light on the nature of the melting transition for the 2D FLL which 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 [22]. A recent extensive Monte Carlo simulation found a first order transition at a temperature close to the estimated one assuming a KT melting transition [23]. After all, it is possible that the nature of the melting transition in 2D strongly depends on the particular conditions and details of the studied specimen which in turn translate into different values of $\xi/a$.

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[1] G. Blatter, M.V. Feigelman, V.B. Geshkenbein, A.I. Larkin and D. Vinokur, Rev. Mod. Phys. \textbf{66}, 1125 (1994) and references therein.
[2] V.L. Berezinskii, Sov. Phys. JETP \textbf{34}, 610 (1972).
[3] J.M. Kosterlitz and D.J. Thouless, J. Phys. \textbf{C6}, 1181 (1973)
[4] M. R. Beasley, J.E. Mooij and T.P. Orlando, Phys. Rev. Lett. \textbf{42}, 1165 (1979).
[5] S. Doniach and B.A. Huberman, Phys. Rev. Lett. \textbf{42}, 1169 (1979).
[6] A.F. Hebard and A.T. Fiory, Phys. Rev. Lett. \textbf{50}, 1603 (1983).
[7] J. Corson, R. Mallozzi, J. Orenstein, J.N. Eckstein and I. Bozovic, Nature \textbf{398}, 221 (1999).
[8] A. Jonsson, P. Minnhagen and M. Nylen, Phys. Rev. Lett. \textbf{70}, 1327 (1993).
[9] E. Domany, M. Schick and R. Swendsen, Phys. Rev. Lett. \textbf{52}, 1535 (1984).
[10] J. E. van Himbergen, Phys. Rev. Lett. \textbf{53}, 5 (1984).
[11] P. Minnagen and M. Wallin, Phys. Rev. \textbf{B36}, 5620 (1987).
[12] S. E. Korshunov, Phys. Rev. \textbf{B46}, 6615 (1992).
[13] D. Bormann and H. Beck, Jour. Stat. Phys. \textbf{76}, 361 (1994).
[14] M. N. Barber, Phys. Rep. \textbf{59}, 375 (1980).
[15] In fact this is the usual parameterization in lattice quantum field theory for the Euclidean action; see for instance K. Jansen, J. Jersak, C.B. Lang, T. Neuhaus and G. von E, Nucl. Phys. \textbf{B 265}, 129 (1986).
[16] M.E. Fisher, M.N. Barber and D. Jasnow, Phys. Rev. \textbf{A8}, 1111 (1973).
[17] An analogous expression for the case of a granular superconductor appears in C. Ebner and D. Stroud, Phys. Rev. \textbf{B28}, 5053 (1983). In a similar way is calculated the orbital magnetic susceptibility, see for instance: A. Sewer, H. Beck, X. Zotos; Physica \textbf{C 317-318}, 475 (1999).
[18] We measured both $E_c$ and $v$ for different values of $\xi$ at $T \sim T_c$ from below and found that the entropic factor fits in well with $v$ in the intermediate range of $\xi$ while the energetic factor is the dominant one when $\xi \sim 1$ and $v$ becomes neglegible.
[19] H. Beck and P. Curty accepted for publication in Physical Review Letters.
[20] Formulas (87) and (88) of \cite{13}, connecting $(\xi, T)$ with $(T_{CG}, z_{CG})$, provide a link between our calculations and Minnhagen phase diagram. However, one should not compare directly values of $(\lambda, K)$ to $(T_{CG}, z_{CG})$, since the former are initial model parameters and the latter vary during renormalization according to the curves shown in B-B figure 6.
[21] Ch. Leeman et al, Phys. Rev. Lett. \textbf{64}, 3082 (1990).
[22] K.J. Strandburg, Rev. Mod. Phys. \textbf{60}, 161 (1988).
[23] Y. Kato and N. Nagaosa, Phys. Rev. \textbf{B47}, 2932 (1993).