A paradigmatic example of a phase transition taking place in the absence of symmetry-breaking is provided by the Berezinskii-Kosterlitz-Thouless (BKT) transition in the two-dimensional XY model. In the framework of canonical ensemble, this phase transition is defined as an infinite-order one. To the contrary, by tackling the transitional behavior of the two dimensional XY model in the microcanonical ensemble, we show that the BKT phase transition is of second order. This provides a new example of statistical ensemble inequivalence that could apply to a broad class of systems undergoing BKT phase transitions.

Landau’s phenomenological theory associates the occurrence of a phase transition with a symmetry-breaking mechanism, detected by the temperature dependence of an order parameter. However, there are many systems undergoing phase transitions in the absence of symmetry-breaking, among the others, this is the case of systems with local symmetries, like gauge systems [1], liquid-gas phase transition, and the broad and important family of Berezinkii-Kosterlitz-Thouless (BKT) phase transitions [2–9].

Recently, in the framework of microcanonical ensemble, Qi and Bachmann [10] have proposed a new classification of phase transitions through the analysis of the inflection point of the microcanonical entropy and of its derivatives. Let us remark that when statistical ensembles are inequivalent the microcanonical ensemble is the only reliable one [11–13]. The aim of the present paper is to characterize and classify the BKT phase transition of the 2D-XY model in the microcanonical ensemble using two different and complementary approaches, that is, resorting to an extended microcanonical classification à la Ehrenfest [14], and following the classification scheme developed by Qi and Bachmann. This is obtained by numerically studying the Hamiltonian dynamics of the model because the invariant measure of a Hamiltonian flow is the microcanonical one. Surprisingly, as we will see, the BKT transition turns out to be a second order transition. This contrasts the commonly accepted classification of BKT transition as being of infinite order. Actually, in the canonical ensemble framework, the spatial correlation length is found to diverge as $\xi \propto e^{\sqrt{T-T_c}}$ at the transition point $T = T_c$ whereas the free energy remains analytic, whence, this is considered an infinite-order transition.

The 2D-XY model is a vector system on a 2-dimensional lattice $\Lambda^2 \subset \mathbb{Z}^2$ where each unit-vector $s_i = (s_{ix}, s_{iy}) = (\cos \theta_i, \sin \theta_i)$ is associated to each site $i \in \Lambda^2$. The standard Hamiltonian for this model is

$$H_{\text{std}}(\theta) = -J \sum_{(i,j)=1}^N s_i \cdot s_j$$

$$= -J \sum_{i,j \in \Lambda^2} \cos (\theta_i - \theta_j), \quad (1)$$

where $(i,j)$ stands for all the pairs of nearest neighbors (thus describing short-range interactions) and $J$ is the coupling constant. Such a model can be regarded as a generalization of the Ising model [15] in the sense that the Ising spins can rotate in two dimensions instead of pointing only in two opposite directions. In this work we add a standard quadratic kinetic energy term of the conjugate momenta $p_i$ to the potential function in Eq. (1). The constant $2NJ$ is also added to the Hamiltonian so that the low energy limit of the potential function is well approximated by the potential energy of a set of coupled harmonic oscillators. This extended Hamiltonian reads as

$$H(p, \theta) = \sum_{i=1}^n \sum_{j=1}^n \frac{p_{(i,j)}^2}{2} + J \left[ \cos(\theta_{(i,j)} - \theta_{(i,j+1)}) + \cos(\theta_{(i,j)} - \theta_{(i+1,j)}) - 2 \right], \quad (2)$$
which is considered with periodic boundary conditions. We have \(N = (n \times n)\). According to Noether’s theorem \([16, 17]\), this system has two first integrals, the total energy \(H(p, \theta) = E\) and the total momentum \(P(p) = \sum_{i \in A} p_i\) associated to the global O(2) symmetry \(\theta_i \rightarrow \theta_i + \alpha\). Geometrically, this can be explained by the confinement of the Hamiltonian dynamics of the system in a hypersurface of fixed energy and fixed total momentum, that is \(\Sigma_{E, \mathcal{P}} = \{x \in \Gamma \mid P(x) = \mathcal{P} \text{ and } H(x) = E\}\), where \(\Gamma\) is the phase space and \(\text{dim}(\Gamma) = 2 (n \times n)\). The only way of tackling the BKT transition on the basis of the Hamiltonian in equation (1) is through the canonical statistical ensemble. Whereas, by rewriting the model Hamiltonian as in equation (2), one allows to tackle the same BKT transition in the microcanonical statistical ensemble. In fact, the invariant measure of the phase space flow associated to this nonintegrable Hamiltonian is the microcanonical measure. It follows that the microcanonical partition function according to the Boltzmann prescription reads

\[
\Omega(E, \mathcal{P}) = \int_\Gamma \delta(H - E) \delta(P - \mathcal{P}) \prod_{i=1}^{N} dp^i \wedge dq^i.
\]

Accordingly, the specific entropy reads

\[
S(\varepsilon, \mathcal{P}) = \frac{1}{N} \ln \left( \frac{\Omega(N \varepsilon, \mathcal{P})}{\Omega_0} \right), \quad (3)
\]

where \(\Omega_0\) is an arbitrary constant, and \(\varepsilon = E/N\) is the specific energy.

In what follows we choose to fix \(\Omega_0 = 1\) and set for simplicity, but without loss of generality, the total momentum equal to zero, that is \(\mathcal{P} = 0\). To simplify the notation, we omit the total momentum fixed to zero in both the argument of microcanonical entropy \(S(\varepsilon, 0) \rightarrow S(\varepsilon)\) and of the microcanonical partition function \(\Omega(E, 0) \rightarrow \Omega(E)\).

Gross [18] was among the first to propose in the 90’s a classification of phase transitions in the microcanonical ensemble based on the change of the curvature of the entropy as a function of the conserved quantity. This idea was refined by Qi and Bachmann [19], where they proposed a definition for a \(k\)-th order phase transition in the microcanonical ensemble through the analysis of the inflection point of \(S(E)\) and of its derivatives. Their classification specified that the occurrence of the second order phase transition is characterized by an inflection point in the first derivative of \(S(E)\). Whereas a first order phase transition is characterized by an inflection point in \(S(E)\). This is physically sound because a first order phase transition is characterized by the presence of latent heat, and this can be explained by the energy gap in the finite-\(N\) pattern of \(S(E)\) which, in the thermodynamic limit, turns into an inflection point [12, 19, 20].

More generally, a phase transition of even order \(2k\) (\(k\) is a positive integer) is associated with an inflection point in the \((2k - 1)\)th derivative of \(S(E)\), and the corresponding negative-valued maximum in the \((2k)\)th derivative of \(S(E)\). Analogously, a phase transition of odd order \((2k - 1)\) occurs if there is an inflection point in the \((2k - 2)\)th derivative of \(S(E)\), and the corresponding minimum in the \((2k - 1)\)th derivative of \(S(E)\) is positive. This is summarized in the following table, where \(S^{(m)}\) denotes the \((m)\)-th derivative of \(S\).

| \((2k-1)\)-th order PT | \((2k)\)-th order PT |
|------------------------|----------------------|
| \(S^{(2k-1)} > 0\)    | \(S^{(2k)} < 0\)    |
| \(S^{(2k)} = 0\)      | \(S^{(2k+1)} = 0\)  |
| \(S^{(2k+1)} > 0\)    | \(S^{(2k+2)} < 0\)  |

TABLE I. Summary of the classification scheme of phase transitions adopted in the present work.

In what follows, we compute the derivatives of the entropy, with respect to the energy, up to 3-th order. In Ref. [21] a method is presented that allows to derive the expressions of the derivatives of the microcanonical entropy and of thermodynamic observables when the only constraint is the fixed total energy of the system \(H = E\). In Ref. [22], it has been shown how to further develop and apply this technique to the case where, besides the total energy of the system, the total momentum \(P\) is also conserved and set equal to zero. Thus, according to Ref. [22], the first three derivatives of the entropy are

\[
\frac{\partial S}{\partial \varepsilon} = \left( \frac{1}{2} - \frac{3}{2N} \right) \langle \kappa^{-1} \rangle_{\mu c} \quad (4)
\]

\[
\frac{\partial^2 S}{\partial \varepsilon^2} = N \left[ \left( \frac{1}{2} - \frac{3}{2N} \right) \left( \frac{1}{2} - \frac{5}{2N} \right) \langle \kappa^{-2} \rangle_{\mu c} + \left( \frac{1}{2} - \frac{3}{2N} \right)^2 \langle \kappa^{-1} \rangle_{\mu c}^2 \right] \quad (5)
\]
\[ \frac{\partial^3 S}{\partial \varepsilon^3} = -N^2 \left[ \frac{1}{2} - \frac{3}{2N} \right] \left( \frac{1}{2} - \frac{5}{2N} \right) \left( \frac{1}{2} - \frac{7}{2N} \right) \langle \kappa^{-3} \rangle_{\mu_c} + \\
- 3 \left( \frac{1}{2} - \frac{3}{2N} \right)^2 \left( \frac{1}{2} - \frac{5}{2N} \right) \langle \kappa^{-1} \rangle_{\mu_c} \langle \kappa^{-2} \rangle_{\mu_c} + \\
+ 2 \left( \frac{1}{2} - \frac{3}{2N} \right)^3 \langle \kappa^{-1} \rangle_{\mu_c}^3 \right], \tag{6} \]

where \( \kappa \) is the specific kinetic energy and \( \langle \cdot \rangle_{\mu_c} \) is the microcanonical average. In what follows, we have adopted the integration algorithm and the initialization of the system performed in Ref. [23], where a geometrical characterization of the BKT phase transition in the microcanonical framework - described by the Hamiltonian in Eq. [2] - was investigated. The microcanonical averages are calculated considering the arithmetic average of the time averages along all the trajectories, that is, if \( A_i(t) \) is the value of the observable \( A \) at the \( i \)th step along the \( j \)th trajectory, its microcanonical average is

\[ \langle A \rangle_{\mu_c} = \frac{1}{N_{traj}} \sum_{j=1}^{N_{traj}} \left( \frac{1}{N_{step}} \sum_{i=1}^{N_{step}} A_i(t) \right), \tag{7} \]

where \( N_{traj} \) is the number of trajectories and \( N_{step} \) is the number of integration steps. The results obtained have very small fluctuations so that in the figures that follow, error bars are not shown because are always smaller than the size of the symbols. In Figure 1 the result of the temperature \( T = (\partial S / \partial \varepsilon)^{-1} \) as a function of the specific energy for \( N = 70 \times 70 \) has been reported. We observe that the curve shows an inflection point in correspondence of \( \varepsilon_c = 1.25 \).

According to the classification scheme of phase transitions in the microcanonical ensemble given by Qi and Bachmann in Table I this inflection point signals already the presence of a phase transition which could be of second order. The results of the second derivative of the entropy for \( N = 10 \times 10 \), \( N = 40 \times 40 \) and \( N = 70 \times 70 \) are displayed in Figure 2. We notice that the non-decreasing property of the caloric curve - equal to the inverse of the first derivative of the entropy - corresponds to a negative second order derivative of \( S(\varepsilon) \), and the inflection point of the same caloric curve at the transition point \( \varepsilon_c \) corresponds to the vanishing of the third derivative of \( S(\varepsilon) \), reported in Figure 3 for \( N = 10 \times 10 \), \( N = 40 \times 40 \) and \( N = 70 \times 70 \). Finally, the decreasing behavior of this derivative below the transition point means that \( \partial^2 S(\varepsilon) < 0 \). Thus, according to Qi and Bachmann classification (table I), the 2D-XY model undergoes a second order phase transition. This result is at odds with the current knowledge about the infinite order character of the BKT phase transition. However, the inequivalence of statistical ensembles has already been found in a broad variety of physical systems [14, 24, 27]. And, as a matter of fact we are here providing a new instance of ensemble inequivalence. The lack of a symmetry-breaking mechanism...
at the grounds of the BKT transition, and thus the lack of a bifurcation pattern of an order parameter to identify the phase transition point may induce some ambiguity in characterizing a sharp transition point. Physically, the transition is characterized by the decoupling of the spin vortex pairs but this can be detected differently in the canonical and microcanonical ensembles, as is discussed in Ref. [28].

Finally, as is well known, Ehrenfest’s classification of phase transitions in the canonical ensemble, based on the order of the free energy derivative which is singular, encountered a major difficulty after Onsager’s rigorous solution of the 2D Ising model. In fact, the divergence of the specific heat in presence of a second order transition entails a singularity of the first derivative of the free energy. However, in the framework of microcanonical ensemble, a coherent classification of phase transitions à la Ehrenfest is possible [14] where a discontinuity in the \((k+1)\)th derivative of the entropy defines a \(k\)th order transition. This approach is in some sense complementary and in tight agreement with the classification proposed by Qi and Bachmann. The presence of the inflection point of the calorific curve at the transition point, in Figure 1, is coherent with the development of an angular point at \(\varepsilon_c\) in the \(\varepsilon\)-pattern of \(\partial^2_S S(\varepsilon)\) at increasing \(N\) as shown in Figure 2 with

\[
\lim_{N \to +\infty} \lim_{\varepsilon \to \varepsilon_c^+} \partial^3_S S = 0 \quad \lim_{N \to +\infty} \lim_{\varepsilon \to \varepsilon_c^-} \partial^3_S S > 0.
\]

Moreover, the \(\varepsilon\)-pattern of \(\partial^2_S S(\varepsilon)\) reported in Figure 2 suggests the presence of an angular point at the transition energy \(\varepsilon_c\) which would entail a discontinuity of \(\partial^2_S S(\varepsilon)\). Figure 3 is compatible with the development of such a discontinuity at increasing \(N\). However, in order to ascertain that this is actually the case, we have resorted to an auxiliary function related to the expression of the specific entropy [3]

defined as a specific volume \(\rho(\varepsilon)\) given by

\[
\rho(\varepsilon) = \left[ \frac{\Omega(N\varepsilon)}{\Omega(N\varepsilon_{\min})} \right]^{1/N},
\]

where \(\Omega(N\varepsilon_{\min})\) is the microcanonical volume at the lowest value of the specific energy \(\varepsilon\) so that \(\rho(\varepsilon_{\min}) = 1\). Introducing the specific volume \(\rho\), the microcanonical specific entropy reads

\[
S(\varepsilon) = \log \rho(\varepsilon),
\]

from which we have

\[
\frac{\partial S}{\partial \varepsilon} = \frac{\partial \rho}{\partial \varepsilon} \rho.
\]

The last expression allows to derive \(\rho\) by the numerical integration of the function \(\partial_S S\), i.e.

\[
\rho(\varepsilon) = \rho(\varepsilon_{\min}) \exp \left[ \int_{\varepsilon_{\min}}^{\varepsilon} \frac{\partial S}{\partial \varepsilon}(\varepsilon) \, d\varepsilon \right].
\]

The derivatives of \(\rho\) with respect to the specific energy \(\varepsilon\) can be obtained deriving equation (9), yielding

\[
\frac{\partial \rho(\varepsilon)}{\partial \varepsilon} = \rho(\varepsilon) \frac{\partial S}{\partial \varepsilon}
\]

\[
\frac{\partial^2 \rho(\varepsilon)}{\partial \varepsilon^2} = \rho(\varepsilon) \left[ \frac{\partial^2 S}{\partial \varepsilon^2} + \left( \frac{\partial S}{\partial \varepsilon} \right)^2 \right]
\]

\[
\frac{\partial^3 \rho(\varepsilon)}{\partial \varepsilon^3} = \rho(\varepsilon) \left[ \frac{\partial^3 S}{\partial \varepsilon^3} + 3 \frac{\partial S}{\partial \varepsilon} \frac{\partial^2 S}{\partial \varepsilon^2} + \left( \frac{\partial S}{\partial \varepsilon} \right)^3 \right].
\]

The third derivative of the specific volume, reported in Figure 4 for \(N = 6 \times 6, N = 10 \times 10, N = 20 \times 20, N = 40 \times 40\) and \(N = 70 \times 70\), is computed through the formula given in Eq. (14). The \(\varepsilon\)-patterns, reported in this figure, clearly show their steepening at increasing \(N\), that is, the formation of a jump. From the results reported in Figures 1 and 2 we know that \(\partial_S S\) and \(\partial^2_S S\) are continuous, therefore, from Eq. (14) we clearly see that any loss of analyticity of \(\partial^2 \rho\) due to the formation of a jump would have its origin in the loss of analyticity of \(\partial^3_S S\). And, according to the classification scheme à la Ehrenfest in the microcanonical ensemble [14], this signals a phase transition of a second order, which is in agreement with

![Figure 3](image-url)
In conclusion, by resorting to the study of the paradigmatic model undergoing a BKT phase transition, that is, the two dimensional XY model, we have found a new kind of statistical ensemble inequivalence. In fact, while in the canonical ensemble the BKT transition is defined as an infinite order transition, we have shown that in the framework of microcanonical ensemble it has the properties typical of a second order phase transition. This is the outcome of an analysis performed by means of two different and complementary approaches developed in the microcanonical ensemble, the Qi and Bachmann approach, and the approach à la Ehrenfest.

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FIG. 4. Third derivative of the specific volume versus energy density for \( N = 6 \times 6 \) (purple circles), \( N = 10 \times 10 \) (blue circles), \( N = 20 \times 20 \) (orange circles), \( N = 40 \times 40 \) (green circles) and \( N = 70 \times 70 \) (red circles). The vertical dotted line marks the transition point at \( \varepsilon_c = 1.25 \).

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[1] S. Elitzur, Physical review d 12, 3978 (1975).
Monthly Notices of the Royal Astronomical Society 328, 339 (2001).

[28] J. Tobochnik and G. Chester, Physical Review B 20, 3761 (1979).

[29] R. Gupta, J. DeLapp, G. G. Batrouni, G. C. Fox, C. F. Baillie, and J. Apostolakis, Physical review letters 61, 1996 (1988).

[30] R. Gupta and C. F. Baillie, Physical Review B 45, 2883 (1992).

[31] P. Jakubczyk and A. Eberlein, Physical Review E 93, 062145 (2016).

[32] J. M. Kosterlitz, Reviews of Modern Physics 89, 040501 (2017).