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Self-consistent harmonic approximation with non-local couplings

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Abstract

We derive the self-consistent harmonic approximation for the $2D$ XY model with non-local interactions. The resulting equation for the variational couplings holds for any form of the spin-spin coupling as well as for any dimension. Our analysis is then specialized to power-law couplings decaying with the distance r as $\propto 1/r^{2+\sigma}$ in order to investigate the robustness, at finite σ, of the Berezinskii-Kosterlitz-Thouless (BKT) transition, which occurs in the short-range limit $\sigma \to \infty$. We propose an ansatz for the functional form of the variational couplings and show that for any $\sigma > 2$ the BKT mechanism occurs. The present investigation provides an upper bound for the lower critical threshold $\sigma^* = 2$, above which the traditional BKT transition persists in spite of the LR couplings.

1 Introduction

Among the different strategies commonly employed to study interacting systems, one that is often used – in its simplest form – is based on the determination of the non-interacting model that better approximates, in a variational sense, the initial, interacting problem. This method, referred to as the Self-Consistent Harmonic Approximation (SCHA), can be improved by considering non-quadratic, but solvable, approximations of the problem at hand or by an integration of the quantum fluctuations to determine an optimized classical potential [1, 2]. Then, the SCHA and its variants may take different forms both for classical or quantum models, and for equilibrium or dynamical properties. They are in general based on the variational principle of the minimization of the energy (or free energy) difference between the interacting model and the approximating one, calculated using the state of the latter [3]. When the approximating model is non-interacting, this approach cannot be used to determine non-trivial correlation functions or interference effects, but also in this case SCHA provides estimates for the equilibrium free energy and the properties of the phases of the model under study. SCHA and its variants, including the so-called pure quantum SCHA, have been as well used to provide an estimate of the quantum corrections to the free energy of nonlinear systems [4, 5] and it has proven useful in several contexts, ranging from the study of phonon spectra in metals and insulators (see [6] and refs. therein) to quantum antiferromagnets [7] and arrays of Josephson junctions [8].

A context in which SCHA has been widely employed along the years is provided by the two-dimensional XY model, where the celebrated Berezinskii-Kosterlitz-Thouless (BKT) transition takes place [9–11]. In the BKT transition, the low temperature phase features vortex-antivortex pairs and power-law correlation functions (with temperature-dependent exponents), while in the high temperature phase topological charges can freely propagate leading to exponential decay in the correlation functions [12–15]. The superfluid density exhibits a universal jump at the critical temperature T_{BKT} [16] and, correspondingly, both the critical exponent η [10, 11] and the power law exponent for the finite size scaling of the largest eigenvalue of the one-body density matrix [17], jump at T_{BKT} from a finite value, respectively 1/4 and 7/8, to zero.

The Hamiltonian of the short-range, nearest-neighbor XY model reads

$$H = -\frac{J_0}{2} \sum_{\mathbf{i},\mathbf{j}} \cos(\theta_{\mathbf{i}} - \theta_{\mathbf{j}}), \tag{1}$$

where J_0 is the coupling constant and the sum is on all the pairs of nearest-neighbor sites of a $2D$ square lattice, on which the variables θ_i are defined. The temperature T_{BKT} of the XY model (1) has been the subject of considerable work, and the value determined by Monte Carlo simulations is given by $k_B T_{BKT}/J_0 = 0.893 \pm 0.001$ [18–23], with k_B the Boltzmann constant. We will put, as usual, $\beta = 1/k_B T$, with T the temperature.

The SCHA for the short-range Hamiltonian (1) applies in a particularly transparent way. One introduces the quadratic Hamiltonian $H_0 = \frac{\tilde{J}_0}{4}\sum_{\mathbf{i},\mathbf{j}}(\theta_\mathbf{i} - \theta_\mathbf{j})^2$ and then variationally determines $\tilde{J}_0$ as a function of J_0 and T, or – equivalently – the dimensionless coupling $\beta\tilde{J}_0$ as a function of βJ_0 [24–27]. It is found that $\tilde{J}_0$ is different from zero for T smaller than a temperature, denoted by T_c, at which the effective $\tilde{J}_0$ drops to zero [24]. An improved determination of the BKT critical temperature T_{BKT} can be obtained inserting $\tilde{J}_0(T)$ in the Nelson-Kosterlitz condition [16] at the BKT critical point [25, 26]. An advantage of this approach is that it can be extended to the quantum phase model [8, 28, 29] describing arrays of Josephson junctions [30, 31] and ultracold bosons in optical lattices in the large filling limit [32].

When the couplings are non-local, i.e. the spins in sites $\mathbf{i}$ and $\mathbf{j}$ are coupled with a strength $J(\mathbf{i}, \mathbf{j})$, the application of the SCHA with the introduction of a variational coupling matrix $\tilde{J}(\mathbf{i}, \mathbf{j})$ faces with the practical problem of solving the full set of conditions for the $\tilde{J}$'s. Here, we focus on the case of Hamiltonians with non-local couplings, proposing and discussing the consequences of a functional ansatz for the variational couplings $\tilde{J}(\mathbf{i}, \mathbf{j})$. In particular, we will consider the case of the $d = 2$ XY with power-law couplings $J(\mathbf{i}, \mathbf{j})$ decaying asymptotically as $J \sim 1/|\mathbf{i} - \mathbf{j}|^{2+\sigma}$. The reason for this choice is three-fold.

i) The nearest-neighbor $2D$ XY model has been extensively studied with SCHA [24–27] providing a benchmark for the short-range limit of the theory. *ii)* The study of statistical mechanics models with long-range interactions attracted considerable attention along the last few decades (see the reviews [33–35]). The general result is that exists a value of the exponent of the power-law decay, denoted by σ^*, such that for $\sigma > \sigma^*$ the universality class is the same of the short-range limit $\sigma \to \infty$. A first derivation by Sak, focusing on $O(n)$ models [36], provided the result $\sigma^* = 2 - \eta_{SR}$, where η_{SR} is the anomalous dimension of the short-range ($\sigma \to \infty$) limit. The validity of this result has been thoroughly investigated using a variety of techniques [37–47], yielding very strong evidences in its favor. Nevertheless, Sak's result only concerns second-order phase transitions, while the BKT transition is an infinite order one, so that the traditional $\sigma^* = 2 - \eta_{SR}$ threshold does not apply to the XY model with non-local couplings. *iii)* Results on the BKT transition for the $2D$ XY model with non-local couplings are very rare, to the best of our knowledge, with exceptions coming from related models such as $1D$ quantum XXZ spin models with long-range interactions [48–50] and random-dilute graphs [51]. Then, qualitative information coming from the SCHA may provide insights for further investigations.

2 SCHA with non-local couplings

We consider the XY model on a 2-dimensional square lattice of N sites with non-local couplings

$$\beta H \equiv -\frac{1}{2}\sum_{\mathbf{i},\mathbf{j}} J(r)\cos(\theta_\mathbf{i} - \theta_\mathbf{j}). \tag{2}$$

where $r = |\mathbf{r}|$ and $\mathbf{r} = \mathbf{i} - \mathbf{j}$ and, as previously mentioned, we choose

$$J(r) = \frac{J}{r^{2+\sigma}}, \tag{3}$$

with $\sigma > 0$. In Eq. (2) we are setting $J \equiv \beta J_0$ and we take energy in units of J_0 (restoring J_0 when useful for clarity).

However, for the moment we do not need to fix a specific form for the couplings $J(r)$, and our results till Eq. (20) hold for any non-local couplings $J(r)$.

Proceeding according to the SCHA, we replace the cosine in the original Hamiltonian (2) with a quadratic term

$$\beta H_0 = \frac{1}{4}\sum_{\mathbf{i},\mathbf{j}} \tilde{J}(\mathbf{r})(\theta_\mathbf{i} - \theta_\mathbf{j})^2 \tag{4}$$

where $\tilde{J}(\mathbf{r})$ is a generic function that has to be determined in a self-consistent way, in order to approximate the original Hamiltonian at best. One may wonder whether the the asymptotic behavior of $\tilde{J}(\mathbf{i})$ can be different from that of $J(r)$, thus it is convenient to derive the self-consistent equations in the most general setting.

To further proceed, we introduce the partition function of the quadratic model

$$Z_0 = \int \prod_{\mathbf{j}} d\theta_{\mathbf{j}} e^{-\beta H_0}, \tag{5}$$

and the corresponding free energy F_0 defined by $Z_0 = e^{-\beta F_0}$. The average on the corresponding Boltzmann measure is defined as

$$\langle \cdot \rangle_0 = \frac{1}{Z_0} \int \prod_{\mathbf{j}} d\theta_{\mathbf{j}} e^{-\beta H_0}. \tag{6}$$

In agreement with the variational principle [3] the best possible result for the couplings $\tilde{J}$ is obtained by minimizing the quantity

$$\mathcal{F} = \beta F_0 + \beta \langle H \rangle_0 - \beta \langle H_0 \rangle_0 \tag{7}$$

with respect to $\tilde{J}(\mathbf{r})$. The equipartition theorem implies that $\langle H_0 \rangle_0 = \frac{N}{2\beta}$, so that this term can be ignored. On the other hand:

$$\begin{aligned} \beta \langle H \rangle_0 &= -\frac{1}{2} \sum_{\mathbf{i},\mathbf{j}} J(|\mathbf{i}-\mathbf{j}|) \langle \cos(\theta_{\mathbf{j}} - \theta_{\mathbf{j}}) \rangle_0 \\ &= -\frac{N}{2} \sum_{\mathbf{r}} J(r) e^{-\frac{1}{2}\left\langle (\theta_0 - \theta_{\mathbf{r}})^2 \right\rangle_0} \end{aligned} \tag{8}$$

where we made use of the identity $\langle \cos A \rangle_0 = e^{-\frac{1}{2}\left\langle A^2 \right\rangle_0}$, valid for every Gaussian measure, and of the translational invariance of the system. Finally, in order to find F_0, and to compute the correlation functions, we have to diagonalize H_0 by means of the Fourier transform. Defining

$$\theta_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{j}} e^{-i\mathbf{q}\cdot\mathbf{j}}\, \theta_{\mathbf{j}}\,; \qquad \theta_{\mathbf{j}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}\in BZ} e^{i\mathbf{q}\cdot\mathbf{j}}\, \theta_{\mathbf{q}} \tag{9}$$

(where the sum on the wavevectors $\mathbf{q}$ is on the first Brillouin zone) we then have

$$\beta H_0 = \frac{1}{2} \sum_{\mathbf{q}\in BZ} K(\mathbf{q}) |\theta_{\mathbf{q}}|^2 \tag{10}$$

where

$$K(\mathbf{q}) = \sum_{\mathbf{r}} \tilde{J}(\mathbf{r}) \Big(1 - \cos(\mathbf{q}\cdot\mathbf{r}) \Big) \tag{11}$$

It follows $Z_0 = (2\pi)^{N/2} \prod_{\mathbf{q}\in BZ} K(\mathbf{q})^{-1/2}$ and

$$\beta F_0 = \frac{1}{2} \sum_{\mathbf{q}\in BZ} \ln K(\mathbf{q}) \tag{12}$$

From Eq. (10) follows that $\left\langle \theta_{\mathbf{q}} \theta_{\mathbf{q}'} \right\rangle_0 = \delta_{\mathbf{q}+\mathbf{q}'} K(\mathbf{q})^{-1}$. Then

$$\begin{aligned} \left\langle (\theta_{\mathbf{0}} - \theta_{\mathbf{r}})^2 \right\rangle_0 &= \frac{1}{N} \sum_{\mathbf{q},\mathbf{q}'\in BZ} \left\langle \theta_{\mathbf{q}} \theta_{\mathbf{q}'} \right\rangle_0 (1 - e^{i\mathbf{q}\cdot\mathbf{r}})(1 - e^{i\mathbf{q}'\cdot\mathbf{r}}) \\ &= \frac{2}{N} \sum_{\mathbf{q}\in BZ} \frac{1 - \cos(\mathbf{q}\cdot\mathbf{r})}{K(\mathbf{q})} \end{aligned} \tag{13}$$

3 Minimization of the free energy

We finally find

$$\mathcal{F} = \frac{1}{2} \sum_{\mathbf{q} \in BZ} \ln K(\mathbf{q}) - \frac{N}{2} \sum_{\mathbf{r}} J(r) e^{-G(\mathbf{r})} \tag{14}$$

with

$$G(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{q} \in BZ} \frac{1 - \cos(\mathbf{q} \cdot \mathbf{r})}{K(\mathbf{q})}. \tag{15}$$

In the lattice case and at generic distance $\mathbf{r}$, the quantity $G(\mathbf{r})$ also depends on the direction of the vector $\mathbf{r}$, but for large distances one may see that it only depends on the modulus r, as expected.

A close inspection of Eq. (14) reveals that the couplings $\tilde{J}(\mathbf{r})$ appear in $\mathcal{F}$ only through the quantities $K(\mathbf{q})$. Then, to proceed with the minimization of $\mathcal{F}$, it is sufficient to derive with respect to the $K(\mathbf{q})$'s, obtaining

$$\frac{\delta \mathcal{F}}{\delta K(\mathbf{q})} = \frac{1}{2K(\mathbf{q})} + \frac{N}{2} \sum_{\mathbf{r}} J(r) \frac{\delta G(\mathbf{r})}{\delta K(\mathbf{q})} e^{-G(\mathbf{r})} \tag{16}$$

and in turn

$$\frac{\delta G(\mathbf{r})}{\delta K(\mathbf{q})} = -\frac{1}{N} \frac{1 - \cos(\mathbf{q} \cdot \mathbf{r})}{K(\mathbf{q})^2}, \tag{17}$$

so that

$$\frac{\delta \mathcal{F}}{\delta K(\mathbf{q})} = \frac{K(\mathbf{q}) - \sum_{\mathbf{r}} J(r) \left[1 - \cos(\mathbf{q} \cdot \mathbf{r})\right] e^{-G(\mathbf{r})}}{2K(\mathbf{q})^2}. \tag{18}$$

Exploiting the definition (11) for $K(\mathbf{q})$ it follows

$$\frac{\delta \mathcal{F}}{\delta K(\mathbf{q})} = \frac{1}{2K(\mathbf{q})^2} \sum_{\mathbf{r}} \mathcal{A}(\mathbf{r}) \Big(1 - \cos(\mathbf{q} \cdot \mathbf{r})\Big), \tag{19}$$

where $\mathcal{A}(\mathbf{r}) \equiv \tilde{J}(\mathbf{r}) - J(r) e^{-G(\mathbf{r})}$, Eq. (19) being valid for each value of $\mathbf{q} \in BZ$ and implying:

$$J(r) = \tilde{J}(\mathbf{r}) e^{G(\mathbf{r})}. \tag{20}$$

Eq. (20) is the desired relation between the couplings $\tilde{J}(\mathbf{r})$ of the optimizing model and the couplings $J(r)$ of the initial model. In solving it, one can actually look for a solution such that the couplings $\tilde{J}$ depend only on r. Eq. (20) has been derived for the $2D$ XY model, but the same calculations can be extended for different dimensions. The same structure of Eq. (20) is found for $O(n)$ models as well. Finally, we notice that Eq. (20) is valid for any non-local form of the couplings $J(r)$, such as the exponential one, and, therefore, it is not limited the power-law decaying form in Eq. (3).

4 Ansatz for the variational couplings

We now come back to the specific problem of the $2D$ XY model with power-law decaying couplings, as defined in Eq. (3): $J(r) = \frac{J}{r^{2+\sigma}}$. We remind that we are setting $J = \beta J_0$ and energy units so that $J_0 = 1$ (unless differently stated).

Within this choice, when the parameter $\sigma \to \infty$, only nearest-neighbor couplings are present, and the Hamiltonian (1) with coupling J_0 between pairs of nearest-neighbors is retrieved. Moreover, we assume $\sigma > 0$ so that the additivity of the thermodynamic quantities is preserved [33, 34]. As recalled in the Introduction, in the short-range limit $\sigma \to \infty$, the system undergoes the BKT transition and this phenomenology is qualitatively captured by the SCHA approximation, in which the original Hamiltonian is replaced with a variational quadratic ansatz. The variational coupling jumps discontinuously to zero at a temperature T_c (see Fig. 1) and provides an estimate for the superfluid stiffness, which can be used in the BKT renormalization group flow equations [24–27].

Our main goal is to discuss the corresponding behavior for finite σ. Without being able to clarify the nature of the universality class and the value of critical exponents, SCHA is nevertheless giving first

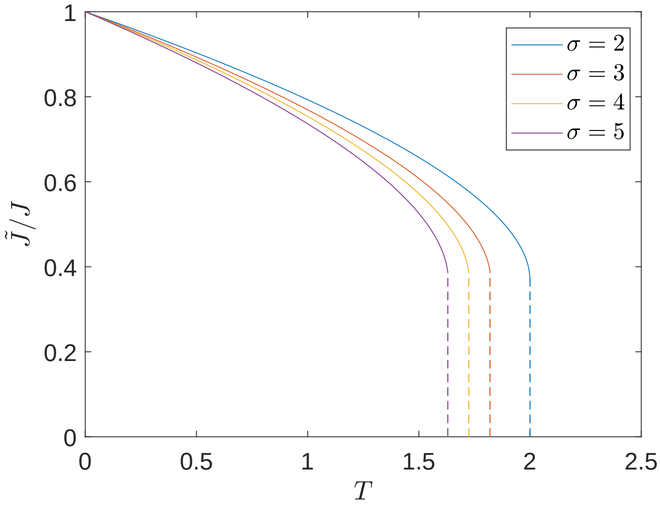

Figure 1: Ratio $\tilde{J}/J$ as a function of $T = 1/J$ for different values of σ. For each σ we find a jump of $\tilde{J}$ to zero at a temperature denoted in the text and in Fig. 2 as T_c.

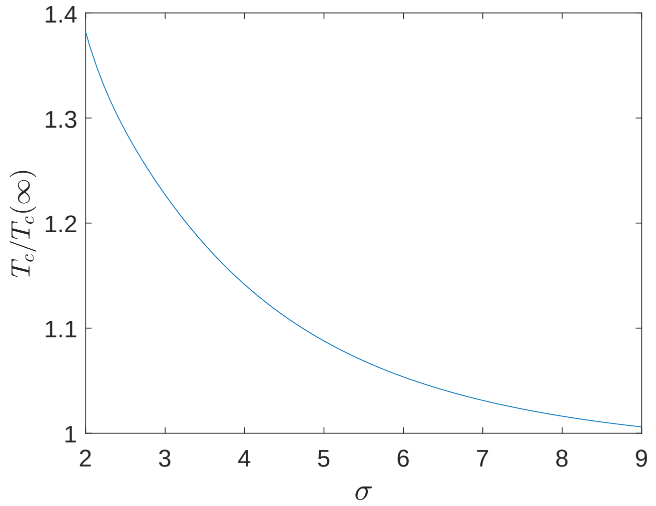

Figure 2: $T_c(\sigma)$ at which $\tilde{J}$ jumps, in units of the $\sigma \to \infty$ value $T_c(\infty) = \frac{4}{e}$. We see that the temperature is finite for $\tilde{\sigma} \to 2$.

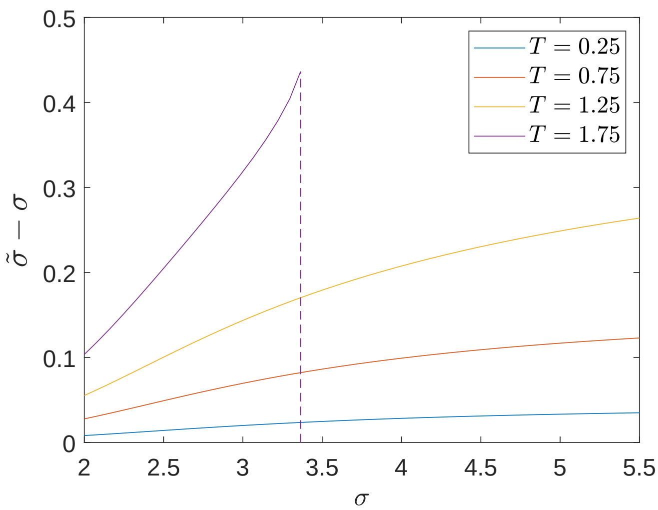

Figure 3: Behavior of $\tilde{\sigma} - \sigma$ as a function of σ for different values of the temperature T. It is seen that $\tilde{\sigma} > \sigma$ everywhere.

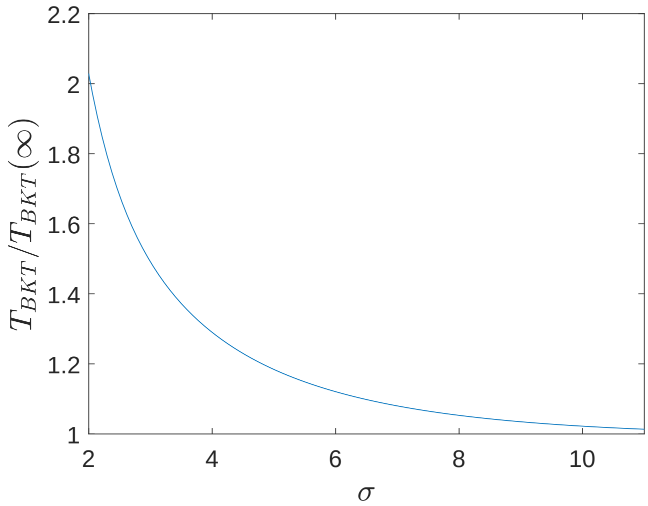

Figure 4: Estimate of $T_{BKT}(\sigma)$ in units of the $\sigma \to \infty$ value $T_{BKT}(\infty)$.

information whether the BKT phenomenology is stable for large σ, as one would expect, and if one can perform an estimate, or – better – put an upper bound for the value of σ^* (defined in this $d = 2$ $O(2)$ case such that for $\sigma > \sigma^*$ one has a BKT transition).

For large σ (i.e. in the short-range limit), the quantity $\langle \cos(\theta_{\mathbf{j}+\mathbf{r}} - \theta_{\mathbf{j}}) \rangle_0 = e^{-G(\mathbf{r})}$ has a temperature-dependent power law behavior. In order to study such temperature dependence in the power-law case, one needs to extract the large distance properties of the variational couplings $\tilde{J}(\mathbf{r})$. Therefore, it is natural to study how a different asymptotic power-law behavior in $\tilde{J}(\mathbf{r})$ with respect to $J(r)$ can actually arise from (20), as anticipated. This lead to the ansatz

$$\tilde{J}(\mathbf{r}) \equiv \frac{\tilde{J}}{r^{2+\tilde{\sigma}}} \tag{21}$$

where $\tilde{\sigma}$ may, in general, be different from σ. Inserting the ansatz (21) in (20), we have to determine $\tilde{\sigma}$ and $\tilde{J}$ as a function of σ and J. We know that in the short-range limit $(\tilde{\sigma}, \sigma \to \infty)$ $\tilde{J}$ as a function of T has a jump from a finite value to zero [24].

An advantage of the ansatz (21) is to give first information about the robustness of the BKT transition from the knowledge of $\tilde{\sigma}$. Indeed, in the short-range nearest-neighbor case, a textbook calculation gives an estimate of T_{BKT} by calculating the energetic and entropic contributions to the free energy ΔF of a free vortex, see e.g. Chapter 4 of [52]. By putting $N = L^2$ and the lattice spacing $\equiv 1$, one has that $\Delta F = \pi J_0 \ln L - k_B T \ln L^2$, giving $k_B T_{BKT} = \pi J_0/2$. A similar situation of competition between the energetic and entropic contributions occurs for the $1D$ Ising model with power-law interactions ($\propto |r|^{-1-\sigma}$), where the excitations are magnetization kinks rather than vortices [53]. In our $2D$ case, one can see that if $\tilde{\sigma} > 2$ then BKT behavior is expected. This can be understood by observing that for $q \to 0$ the scaling of the propagator due to the effective interactions ($\propto 1/q^{\tilde{\sigma}}$) is irrelevant with respect to the one of the free propagator ($\propto 1/q^2$), from which one can conclude the irrelevance of the non-local interaction when $\tilde{\sigma} > 2$. We notice that this is in agreement with the known rigorous result of a low-temperature phase with spontaneous symmetry breaking and magnetization for XY couplings decaying faster than $1/r^4$ in $2D$ [54]. In conclusion, if one finds

$$\tilde{\sigma}(\sigma) > 2, \tag{22}$$

then it is possible to conclude that SCHA is indicating persistence of BKT at that σ.

5 Results

Let us start from the case $\sigma > 2$, deferring our comments on the case $\sigma < 2$ to the end of the present Section. By plugging the ansatz (21) in Eq. (20), we numerically solve for $\tilde{J}$ and $\tilde{\sigma}$ in a square lattice. We considered growing values of N to solve Eq. (20), and we observed that convergence of the result is obtained for $N \sim 10^4$.

In Fig. 1 we show $\tilde{J}/J$ as a function of the temperature for different values of $\sigma \geq 2$. The temperature T_c corresponding to the jump is σ-dependent (see below for a discussion of the difference between T_c and T_{BKT}). In the $\sigma \to \infty$ limit it converges to the short-range value $k_B T_c(\infty) = \frac{4}{e} J_0$ [24]. The behavior of $T_c(\sigma)$ in units of $T_c(\infty)$ is shown in Fig. 2. We found that T_c is a decreasing function of σ which remains finite as σ approaches 2.

Our main result is that one has $\tilde{\sigma} > 2$. This is apparent from Fig 3, where we show the behavior of $\tilde{\sigma} - \sigma$ as a function of σ for different values of the temperature T. This quantity is of course only defined as long as $T < T_c(\sigma)$. In particular, since $T_c(\sigma) \to T_c(\infty)$ as $\sigma \to \infty$, for $T < T_c(\infty)$ the curve is defined for every σ. As expected, $\tilde{\sigma} - \sigma$ is temperature-dependent and $\tilde{\sigma} \to \sigma$ as $T \to 0$. For $T < T_c(\infty)$, as $\sigma \to \infty$, $\tilde{\sigma} - \sigma$ goes to a constant, in agreement with the natural expectation of recovering the short-range result. It is important to notice that, for each value of the parameters, we have that $\tilde{\sigma} > \sigma$ and therefore the validity of the condition (22).

Going to the $\sigma < 2$ case, since T_c is finite for $\sigma \to 2^+$ and also $\tilde{\sigma} > \sigma$, one may be tempted to investigate whether the BKT phase can survive in the $\sigma < 2$ regime, and ascertain if the value of σ for which the long-range tail of the couplings modifies the critical behavior is actually smaller than 2. However, for $\sigma < 2$ the solution of Eq. (20) with $\tilde{J}(\mathbf{r})$ in the form of Eq. (21) is no longer unique. Then, since our ansatz considers only a subspace of the possible functional forms of $\tilde{J}(r)$ and the difference in the energy of the solutions can be of the same order of the error introduced by the ansatz (21), we cannot safely draw any conclusion for $\sigma < 2$. To further explore the $\sigma < 2$ region one has to resort both to the numerical solution of Eq. (20) without the use of the ansatz (21) and to the application of more sophisticated techniques. It is anyway fair to conclude that 2 is an upper bound for σ^*, i.e. for $\sigma > 2$ one has a BKT transition at finite temperature.

6 Estimate of T_{BKT}

$T_c(\sigma)$ can be considered only a very crudest estimate of the temperature at which the universal jump occurs. For the short-range limit, a better estimate of T_{BKT} can be obtained if we define T_{BKT} as the temperature at which the variational $\tilde{J}$ reaches the value $\tilde{J}_{BKT} = \frac{2}{\pi}$ [26]. This value, restoring the temperature, is obtained by considering the Nelson-Kosterlitz condition [16] for the short-range XY model, reading $J_{superfl}/k_B T = 2/\pi$, and using the SCHA value $\tilde{J}_0$ as estimate for the superfluid stiffness $J_{superfl}$. In this way, one can obtain $k_B T_{BKT} = 1.06 J_0$, improving with respect to the value $T_c(\sigma \to \infty)$ (given by $k_B T_c = (4/e) J_0 = 1.47 J_0$). A further improvement could be obtained by using estimates of the dielectric constant in the Nelson-Kosterlitz transition, giving $k_B T_{BKT} = 0.96 J_0$ [26]. These estimates can be compared with the functional renormalization group estimate, $k_B T_{BKT} = 0.94 J_0$ [55], with a (functional) renormalization group calculation using a renormalized initial condition, $k_B T_{BKT} = 0.89 J_0$[56], with the analytic calculation based on the mapping on the $1D$ quantum XXZ model, $k_B T_{BKT} = 0.883 J_0$ [57], and with the previously mentioned Monte Carlo value $k_B T_{BKT} = 0.893 J_0$. We notice that the Nelson-Kosterlitz condition can be used to extract T_{BKT} with high precision from Monte Carlo data [23].

The condition $\tilde{J}_{BKT} = \frac{2}{\pi}$ can be thought as corresponding to the value at which the Gaussian low-temperature theory becomes unstable due to the presence of the topological excitations [10, 11]. This improves the estimate of T_{BKT}, since the plain SCHA does not account for the presence of these excitations, i.e. the real mechanism underlying the transition.

Then, we expect that a better estimate of $T_{BKT}(\sigma)$ can be obtained if we apply the same line of reasoning for finite σ, i.e. using a two-step approach in which SCHA is used to estimate the superfluid stiffness and then the latter is used in the Nelson-Kosterlitz condition. However, with general non-local couplings, and power-law couplings in particular, a microscopic relation between the coupling $J(r)$ and the superfluid stiffness is not known. One can think to use $\tilde{J}$ instead of J, but this would heavily underestimate the effect of the tails of the variational couplings $\tilde{J}$.

We propose to proceed defining the analog of the nearest-neighbors coupling in the context of our variational quadratic Hamiltonian (21). We then make use once again of the variational method to determine the best value of J_{nn} in

$$\beta H_{nn} = \frac{J_{nn}}{2} \sum_{\mathbf{i},\mathbf{j}} (\theta_{\mathbf{i}} - \theta_{\mathbf{j}})^2 \tag{23}$$

which best approximates H_0. We find the result:

$$J_{nn}(\tilde{J},\tilde{\sigma}) = \frac{1}{2N}\sum_{\mathbf{q}\in BZ}\frac{K(\mathbf{q})}{2-\cos q_x-\cos q_y} \tag{24}$$

where $K(\mathbf{q})$ is computed from (11) with $\tilde{J}(r) = \frac{\tilde{J}}{r^{2+\sigma}}$ and $\tilde{J}$, $\tilde{\sigma}$ corresponding to the solutions of the variational equation (20).

We can then find our estimate of T_{BKT} by choosing $\tilde{J} = \frac{1}{T}$ such that $J_{nn} = \frac{2}{\pi}$. The behavior of $T_{BKT}(\sigma)$ in units of the short-range value $T_{BKT}(\infty)$ are shown in Fig. 4. The dependence on σ is stronger than those of $T_c(\sigma)$, even if the qualitative behavior is the same. In particular, $T_{BKT}(\sigma)$ remains finite as well as $\sigma \to 2^+$. Whether this suggests or not the scenario in which the BKT transition survives for $\sigma < 2$ remains open.

7 Conclusions

In this paper we studied the self-consistent harmonic approximation (SCHA) for the $2D$ XY model with non-local couplings. The approach relies on the well known procedure of approximating the interacting model under study with a quadratic model, whose coefficients are optimized minimizing the free energy difference. We derived an equation for the variational couplings which is valid for general non-local interactions and in a form that can be used for other models, such as long-range $O(n)$ models. Then, we focused on power-law couplings $J(r)$ decaying as $J(r) = J/r^{2+\sigma}$.

The short-range limit $\sigma \to \infty$ exhibits the Berezinskii-Kosterlitz-Thouless (BKT) transition. To extract information about the robustness of the BKT transition at finite σ we propose an ansatz for the functional form of the variational couplings $\tilde{J}(r)$ reading $\tilde{J}(r) = \tilde{J}/r^{2+\tilde{\sigma}}$, where $\tilde{J}$ and $\tilde{\sigma}$ have to be determined as a function of J and σ.

The study of this dependence revealed that for $\sigma > 2$ BKT occurs. The critical temperature at which $\tilde{J}$ drops to zero has been determined. We then used the output of the SCHA calculation in the Nelson-Kosterlitz condition at the critical point to obtain an improved estimate of the BKT critical temperature.

Our results suggest that, once the value σ^* is defined in such a way that for $\sigma > \sigma^*$ one has a BKT transition, then one has an upper bound for σ^* given by $\sigma^* = 2$. For $\sigma < 2$ the SCHA has two solutions for the variational parameters. Therefore further work is needed to clarify the structure of the phase diagram and the critical points for $\sigma < 2$.

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