

Finite-Temperature Renormalization Group Analysis of Interaction Effects in 2D Lattices of Bose-Einstein Condensates

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Abstract

By using a renormalization group analysis, we study the effect of interparticle interactions on the critical temperature T_{BKT} at which the Berezinskii-Kosterlitz-Thouless (BKT) transition occurs for Bose-Einstein condensates loaded at finite temperature in a 2D optical lattice. We find that T_{BKT} decreases as the interaction energy decreases; when $U/J = 36/\pi$ one has $T_{BKT} = 0$, signaling the possibility of a quantum phase transition of BKT type.

I. INTRODUCTION

It has been recently suggested [1] that a 2D optical lattice of Bose-Einstein condensates [2] may allow for the observation of a finite-temperature phase transition to a superfluid regime where the phases of the single-well condensates are coherently aligned. In fact, in

an appropriate range of parameters, the thermodynamical properties of the bosonic lattice at finite temperature may be well described by the Hamiltonian of the XY model [1], and, as it is well known, the $2D$ XY model exhibits the Berezinskii-Kosterlitz-Thouless (BKT) transition [3–5]. The BKT phase transition occurs via an unbinding of vortex defects: the low-temperature phase, for T below the BKT temperature T_{BKT} , is characterized by the presence of bound vortex-antivortex pairs and the spatial correlations exhibit a power-law decay. For $T \sim T_{BKT}$ the pairs start to unbind (see e.g. [6,7]): in the high-temperature phase, only free vortices are present, leading to an effective randomization of the phases and to an exponential decay of the correlation functions.

The Hamiltonian describing the properties of bosons in deep optical lattices is the so called Bose-Hubbard Hamiltonian [8], in which two terms are present: a kinetic term describing the hopping of the bosons with tunneling rate t , and a potential term describing the interaction between bosons in the wells of the array with interaction energy U (which is proportional to the s -wave scattering length). The description of bosons in deep lattices by means of the Bose-Hubbard Hamiltonian holds also at finite temperature, provided that the temperature effects do not induce the occupation of higher bands: for a $2D$ optical lattice confined to a plane by a magnetic potential having frequency ω_z , this implies that the Bose-Hubbard Hamiltonian description is valid up to temperatures T such that $\hbar\omega_z \gtrsim k_B T$. When the average number of bosons N_0 per site is high enough and the interaction energy is larger than t/N_0 , one may map - *also at finite temperature* - the Bose-Hubbard Hamiltonian in the quantum phase Hamiltonian [1]: the conjugate variables are the phases and the particle numbers of the condensates in the different sites of the lattice. Thus, also at finite temperature, the phase diagram is determined by the competition of two energies: the Josephson energy $J \approx 2tN_0$, proportional to the tunneling rate between neighbouring sites of the $2D$ square optical lattice, and the interaction energy U . For $U = 0$, the quantum phase Hamiltonian reduces to the XY Hamiltonian, exhibiting then a BKT transition at $T_{BKT} \sim J/k_B$: for $T < T_{BKT}$ the system as a whole behaves as a superfluid with phase coherence across the array. Very accurate Monte Carlo simulations yield, in the thermodynamic

limit, $T_{BKT} = 0.898J/k_B$ [9].

In this paper we determine the effect of the interaction energy U on the BKT transition. When $U \ll J$, a BKT transition still occurs at a critical temperature $T_{BKT}(U)$: we find that $T_{BKT}(U)$ is smaller than T_{BKT} and decreases with U (see Fig. 1). Intuitively speaking, the quantum phase Hamiltonian, as well as the Bose-Hubbard Hamiltonian, in the limit $U \gg J$ describes a Mott insulator, while in the opposite limit, $J \gg U$, the array behaves as a phase-coherent superfluid (e.g., see [10,11]): thus, when U increases, the superfluid region in the phase diagram decreases. Although in two dimensions there is not long-range order at finite temperature due to the Mermin-Wagner theorem, still the system exhibits superfluid behavior for $T < T_{BKT}$ [11]: thus one expects that $T_{BKT}(U)$ should decrease when U increases. We also find (see Section III) that, when U/J is equal to the critical value $(U/J)_{cr} = 36/\pi$, one has that $T_{BKT}(U) = 0$, signaling the possibility of a ($T = 0$) quantum phase transition.

The quantum phase Hamiltonian describes also the behavior of superconducting Josephson networks below the temperature T_{BCS} at which each junction becomes superconducting [11–13]. The momenta conjugate to the phases of the macroscopic wavefunctions of the superconducting grains are the number of Cooper pairs, J is the Josephson energy of the superconducting Josephson junctions and U is the charging energy due to the Coulomb repulsion between Cooper pairs. We observe that, in superconducting Josephson arrays, the interaction term is written in general as $\sum_{ij} U_{ij} N_i N_j$ where N_i is the Cooper pairs number at the site i : U_{ij} is proportional to the inverse of the capacitance matrix and may be also non-diagonal (i.e., $U_{ij} \neq 0$ with $i \neq j$). At variance, for bosons in deep optical lattices, the interaction term is $\sum_i U_{ii} N_i^2$, which corresponds, in a suitable range of parameters, to a *diagonal* quantum phase model.

The analogy between superconducting Josephson networks and atomic gas in deep optical lattices is then clear: in each well of the periodic potential there is a condensate grain, appearing at the Bose-Einstein condensation temperature T_{BEC} . When T_{BEC} is larger than all other energy scales, the atoms in the well i of the 2D optical lattice may be described

by a macroscopic wavefunction. It becomes apparent, then, that an optical network can be regarded as a network of *bosonic* Josephson junctions. Furthermore, in both systems, when the interaction term is neglected respect to the energy associated to the particle hopping, one has that the whole $2D$ array becomes superfluid at the temperature T_{BKT} at which the BKT transition occurs, with T_{BKT} smaller than T_{BCS} for superconducting Josephson networks and smaller than T_{BEC} for bosonic Josephson networks.

The plan of the paper is the following: in Section II we introduce the effective Hamiltonian describing bosons hopping on a deep optical lattice and, by using a semiclassical approximation [14], we compute the effective Josephson energy in presence of the interaction energy U . In Section III we evaluate the effect of the quantum fluctuations on T_{BKT} by putting in the renormalization group equations the effective Josephson energy obtained in Section II; a comparison with previous results is then carried out. Details of the computations skipped in the text are in the Appendix A. Section IV is devoted to some concluding remarks.

II. THE RENORMALIZED JOSEPHSON ENERGY

$2D$ optical lattices are created using two standing waves [2]: when the polarization vectors of the two laser fields are orthogonal, the periodic potential is

$$V_{opt} = V_0[\sin^2(kx) + \sin^2(ky)], \quad (1)$$

where $k = 2\pi/\lambda$ is the wavevector of the lattice beams. V_0 is usually expressed in units of $E_R = \hbar^2 k^2 / 2m$ (where m is the atomic mass): in [2] it is $\lambda = 852\text{ nm}$ and $E_R = h \cdot 3.14\text{ kHz}$. Around the minima of the potential (1) one has $V_{opt} \approx m\tilde{\omega}_r^2(x^2 + y^2)/2$ with

$$\tilde{\omega}_r = \sqrt{\frac{2V_0 k^2}{m}}. \quad (2)$$

When $\tilde{\omega}_r \gg \omega_z$ (with ω_z the frequency of the confining magnetic potential superimposed to the optical potential and acting along z), the system realizes a square array of tubes, i.e. an array of harmonic traps elongated along the z -axis [2].

When all the relevant energy scales are small compared to the excitation energies, one can expand the field operator [8] as

$$\hat{\Psi}(\vec{r}, t) = \sum_i \hat{\psi}_i(t) \Phi_i(\vec{r}) \quad (3)$$

with $\Phi_i(\vec{r})$ the Wannier wavefunction localized in the i -th well (normalized to 1) and $\hat{N}_i = \hat{\psi}_i^\dagger \hat{\psi}_i$ the bosonic number operator. Substituting the expansion of $\hat{\Psi}(\vec{r}, t)$ in the full quantum Hamiltonian, one gets the effective Hamiltonian describing the bosons hopping on the deep optical lattice [8,15]

$$H = -t \sum_{\langle i,j \rangle} (\hat{\psi}_i^\dagger \hat{\psi}_j + h.c.) + \frac{U}{2} \sum_i \hat{N}_i (\hat{N}_i - 1). \quad (4)$$

In Eq.(4) $\sum_{\langle i,j \rangle}$ denotes a sum over all the distinct pairs of nearest neighbours; t and U are respectively the tunneling rate and the interaction energy, and are given by

$$t \simeq - \int d\vec{r} \left[\frac{\hbar^2}{2m} \vec{\nabla} \Phi_i \cdot \vec{\nabla} \Phi_j + \Phi_i V_{ext} \Phi_j \right] \quad (5)$$

and

$$U = \frac{4\pi\hbar^2 a}{m} \int d\vec{r} \Phi_i^4 \quad (6)$$

(a is the s -wave scattering length).

As discussed in the Introduction, one can show that, when V_0 and ω_z are large enough, the system is described by the Hamiltonian (4) up to temperatures $T \sim \hbar\omega_z/k_B$ [1]. Upon defining $J \approx 2tN_0$, the Hamiltonian (4), for $N_0 \gg 1$ and $J/N_0^2 \ll U$ [16], reduces to

$$\hat{H} = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - \frac{U}{2} \sum_i \frac{\partial^2}{\partial \theta_i^2}. \quad (7)$$

For a 2D lattice with V_0 between $20E_R$ and $25E_R$ and $N_0 \approx 170$ as in [2], one sees that the condition $\gg J/N_0^2$ is rather well satisfied and that J/k_B is of order of $20nK$. For $U = 0$, (7) is the XY Hamiltonian:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j). \quad (8)$$

The Hamiltonian (7) describes the so-called quantum phase model [11–13]. There is an huge amount of literature on the properties of $2D$ superconducting Josephson arrays studied by means of the quantum phase model [11–13]. A (not exhaustive) list of relevant papers includes mean-field and coarse-graining approaches [17–19], Monte Carlo results [20–24], renormalization group calculations [14,21] and self-consistent harmonic approximations [21,25,26] (more references are in [11]). In the following we shall study the renormalization-group equations in which it is used an effective value of the Josephson energy computed within the harmonic approximation [14].

The starting point is the partition function Z of the quantum phase model: using the path integral formalism, from (7), one has

$$Z = \int \mathcal{D}\theta e^{-\frac{1}{\hbar}S[\theta]}, \quad (9)$$

where the action S is given by

$$S[\theta] = \int_0^{\hbar\beta} d\tau \left[\frac{\hbar^2}{2U} \sum_j \left(\frac{\partial \theta_j}{\partial \tau} \right)^2 + J \sum_{\langle i,j \rangle} (1 - \cos \theta_{ij}) \right] \quad (10)$$

with $\beta = 1/k_B T$ and $\theta_{ij} \equiv \theta_i - \theta_j$. Separating the phases as $\theta_i(\tau) = \varphi_i + \delta_i(\tau)$, where φ_i is a static vortex configuration and $\delta_i(\tau)$ is a fluctuation about φ_i , the path-integral partition function (9) can be written as

$$Z = \int \mathcal{D}\varphi \mathcal{D}\delta e^{-\frac{1}{\hbar}S[\varphi,\delta]} \quad (11)$$

where

$$S[\varphi,\delta] = \int_0^{\hbar\beta} d\tau \left[\frac{\hbar^2}{2U} \sum_i \dot{\delta}_i^2(\tau) + J \sum_{\langle i,j \rangle} (1 - \cos \varphi_{ij} \cos \delta_{ij}) \right], \quad (12)$$

with $\varphi_{ij} \equiv \varphi_i - \varphi_j$ e $\delta_{ij} \equiv \delta_i - \delta_j$. Assuming that φ_i and δ_i are slowly varying over the size of the array [14,12], i.e.

$$\cos \varphi_{ij} \approx 1 - \varphi_{ij}^2/2 \quad (13)$$

and

$$\cos \delta_{ij} \approx 1 - \delta_{ij}^2/2, \quad (14)$$

one gets

$$Z = Z_0 \int \mathcal{D}\varphi \exp\left\{-\frac{1}{2}\beta\bar{J} \sum_{\langle i,j \rangle} \varphi_{ij}^2\right\}, \quad (15)$$

where $Z_0 \equiv \int \mathcal{D}\delta e^{-\frac{1}{\hbar}S_0[\delta]}$ and

$$S_0[\delta] = \int_0^{\hbar\beta} d\tau \left[\frac{\hbar^2}{2U} \sum_i \dot{\delta}_i^2 + \frac{J}{2} \sum_{\langle i,j \rangle} \delta_{ij}^2 \right]. \quad (16)$$

In Eq.(15) \bar{J} is the renormalized Josephson energy, which is given by

$$\bar{J} \simeq J \left(1 - \frac{1}{2} \langle \delta_{ij}^2 \rangle_0\right) \quad (17)$$

with

$$\langle \delta_{ij}^2 \rangle_0 \equiv \frac{1}{Z_0} \int \mathcal{D}\delta e^{-\frac{1}{\hbar}S_0[\delta]} \delta_{ij}^2. \quad (18)$$

The evaluation of $\langle \delta_{ij}^2 \rangle_0$ can be carried out in a standard way [12] and one has

$$\langle \delta_{ij}^2 \rangle_0 = \sqrt{\frac{\pi U}{J}} \frac{1}{\eta^3} \int_0^\eta x^2 \coth x \, dx \quad (19)$$

where

$$\eta = \beta \sqrt{\pi U J}. \quad (20)$$

III. RENORMALIZATION GROUP EQUATIONS

In the renormalization group equations for the 2D XY model [3–5] the scale-dependent screened charge \mathcal{K} depends on the dimensionless scaling parameter $l = \log(r/a)$ (where r is the vortex distance and a is the lattice spacing) and it is given by $\mathcal{K}(l) = \beta J/\epsilon(l)$, where the dielectric constant $\epsilon(l)$ expresses the screening of the vortex-antivortex interaction due to the presence of other vortices [5]. The renormalization group recursion equations read [5]

$$\frac{d\mathcal{K}^{-1}(l)}{dl} = 4\pi^3 y^2(l) \quad (21)$$

and

$$\frac{dy(l)}{dl} = [2 - \pi\mathcal{K}(l)]y(l) \quad (22)$$

where $y \propto r^2 e^{-\beta V(r)/2} e^{-\beta\mu}$, with $e^{-\beta\mu}$ is the fugacity for creating a vortex pair and $V(r)$ correspond to the screened vortex-antivortex potential. The study of the scaling equations (21)-(22) about the fixed point $y_f = 0$, $\mathcal{K}_f = 2/\pi$ shows that the BKT transition occurs at $2 - \pi\mathcal{K}(l=0) \approx 0$, where $\mathcal{K}(l=0) = \beta J/\epsilon(l=0) = \beta J$ [5].

In presence of the quantum fluctuations, one has to replace the scale-dependent charge $\mathcal{K}(l)$ by $\bar{\mathcal{K}}(l)$ with $\bar{\mathcal{K}}(l=0) = \beta\bar{J}$ and \bar{J} given by Eqs.(17) and (19). Denoting with $T_{BKT}(U)$ the BKT transition temperature for a given U , one finds the following equation for $K \equiv J/k_B T_{BKT}(U)$:

$$F(K) = 2 - \pi K \left(1 - \frac{1}{2\pi^2 X_u K^3} \int_0^{\pi\sqrt{X_u}K} x^2 \coth x \, dx \right) = 0 \quad (23)$$

where $X_u = U/\pi J$.

The root of Eq.(23) indicates the critical point at which a BKT transition occurs. The eventual occurrence of a double root for Eq.(23) might correspond to what is called in literature a *reentrant* behavior. Indeed it has been often argued (see Refs. in the review [11]) that the quantum phase model may undergo at low temperatures a reentrant transition induced by the quantum fluctuations: namely, fixing U/J and lowering the temperature, one could switch from an insulating phase to a superconducting one at $T_{BKT}(U)$ and then, lowering further the temperature, one finds another critical temperature $T^{(1)}(U)$ at which the system comes back (*reenters*) in the insulating phase. Consistent with the reentrant scenario is the dramatic decrease of the specific heat at very low temperatures [20] and, as discussed, the presence of double roots for T_{BKT} in the renormalization group equations.

The phenomenon of the reentrance - although not universal - is a non-perturbative effect: in fact, opposite results may be obtained by means of different truncations for the series

expansion of the function F . For instance, if in Eq.(23) one expands the hyperbolic cotangent as $\coth x \approx 1/x + x/3$, one gets an expression for $F(K)$ which gives two roots for T_{BKT} . If instead, for $\eta < \pi$, one uses the expansion $\coth x = \frac{1}{x} + \sum_{n=1}^{\infty} \frac{2^{2n} B_{2n}}{(2n)!} x^{2n-1}$ where the B_n 's are the Bernoulli numbers [27], one obtains the equation:

$$F(K) = 2 - \pi K \left(1 - \frac{1}{4K} - \sum_{n=1}^{\infty} \frac{6^n 2^{4n} B_{2n} x_u^n K^{2n-1}}{2(2n+2)(2n)!} \right) = 0 \quad (24)$$

with $x_u = \pi U/24J$. Since $B_{4n} < 0$ for $n = 1, 2, \dots$, and $B_{4n+2} > 0$ for $n = 0, 1, 2, \dots$, if one truncates the sum in Eq.(24) to the $(2n+1)$ -th order with $n = 0, 1, 2, \dots$, one finds $F(K) \rightarrow \infty$ for $K \rightarrow \infty$ and then Eq.(24) has two roots; at variance, if one truncates the sum to the $(2n)$ -th order with $n = 1, 2, \dots$, one finds $F(K) \rightarrow -\infty$ for $K \rightarrow \infty$ and Eq.(24) admits only one root. Thus one cannot truncate the sum in Eq.(24) to any finite order, even for $U/J \ll 1$; the origin of this problem is that the expansion used to get (24) is a series with terms having alternating signs. In addition, to find the roots of the equation $F(K) = 0$ one has to evaluate the integral in (19) up to $\sqrt{UJ}/k_B T_{BKT}$, and, also with U small, η may become large requiring to use all the orders in Eq.(24).

A way to overcome the above mentioned difficulties is to use in Eq.(23) the Mittag-Leffler expansion of the hyperbolic cotangent, i.e. $\pi \coth \pi x = 1/x + 2x \sum_{n=1}^{\infty} (x^2 + n^2)^{-1}$: in this way Eq.(23) can be written as

$$F(K) = 2 - \pi K \left[1 - \frac{1}{4K} - \frac{1}{X_u K^3} g(K, X_u) \right] = 0 \quad (25)$$

where

$$g(K, X_u) \equiv \sum_{n=1}^{\infty} \left[\frac{X_u K^2}{2} - \frac{n^2}{2} \log \left(1 + \frac{X_u K^2}{n^2} \right) \right]. \quad (26)$$

An analytic expression for $F(K)$ valid for $U/J \ll 1$ is given by Eq.(A5) in the Appendix A.

A detailed study of the function $F(K)$ is in the Appendix A. Here we observe that, in the limit $U/J \rightarrow 0$, one finds $2 + \frac{\pi}{4} - \pi K = 0$, from which $K_0 \equiv K(U/J \rightarrow 0) = \frac{8+\pi}{4\pi}$ and $k_B T_{BKT}(0) \simeq 1.128J$. Furthermore, for $U/J < 36/\pi$, one can show (see the Appendix A) that $F(K) \rightarrow -\infty$ for $K \rightarrow \infty$ and that $F'(K) < 0$: since F tends to the positive value

$2 + \pi/4$ for $K \rightarrow 0$, one can safely conclude that, for $U/J < 36/\pi$, Eq.(25) has an *unique* solution. At variance, one can show that, for $U/J > 36/\pi$, Eq.(25) does not admit any solution, while for $U/J = 36/\pi$ one has $K \rightarrow \infty$, i.e. $T_{BKT}(U) \rightarrow 0$. A plot of $F(K)$ and $F'(K)$ for three values of U/J respectively smaller than, equal to and larger than $36/\pi$ is given in Figs. 2 and 3. One may infer that, at $T = 0$, a phase transition is expected to occur at the critical value $(U/J)_{cr} = 36/\pi$: this value is in reasonable agreement with the mean-field estimates for the $T = 0$ transition. In fact, for the diagonal quantum phase model, one has that the mean-field prediction [17,19] is $(U/J)_{cr} \approx 2z = 8$ where $z = 4$ is the number of nearest neighbours.

In Fig. 1 we plot as empty circles the values of $T_{BKT}(U)/T_{BKT}(0)$ as a function of U/J from the numerical solution of Eq.(25). If one uses the analytic expression (A5) for the function $F(K)$ one gets, for $U/J \lesssim 1/2$, an error lesser than 1%. A much better estimate may be obtained by expanding the function $F(K)$ near K_0 : in this way Eq.(25) reads

$$F(K) \approx F(K_0) + (K - K_0) \cdot F'(K_0) = 0,$$

and then

$$K \approx K_0 - \frac{F(K_0)}{F'(K_0)}. \quad (27)$$

In Fig. 1 Eq.(27) is plotted as a solid line.

We may conclude that Eq.(25) admits, for small U/J , a unique solution and this excludes the possibility of reentrant behavior. Of course, our conclusion relies on the approximations (13)-(14) made in order to estimate \bar{J} and $\langle \delta_{ij}^2 \rangle_0$. A more careful treatment accounting for the periodicity of the phases in Eq.(12) seems to be highly desirable to put on a more solid base all the contrasting issues related to the reentrant behavior of the systems described by the Hamiltonians (4) and (7). It is comforting to see that the experimental study of weakly interacting bosons on $2D$ optical networks and the investigations of their superfluidity properties at very low temperatures could provide new insights also on this intriguing and yet poorly understood problem (see also the recent papers [28]).

IV. CONCLUDING REMARKS

In this paper we studied, by means of a renormalization group analysis, the effect of interparticle interactions on the critical temperature at which the Berezinskii-Kosterlitz-Thouless transition occurs for Bose-Einstein condensates loaded in a $2D$ optical lattice at finite temperature. We determined the shift of the Berezinskii-Kosterlitz-Thouless transition temperature induced by the interaction term and we compared our findings with previously known results.

APPENDIX A: PROPERTIES OF THE RENORMALIZATION GROUP EQUATION

In this Appendix we study the properties of the function $F(K)$ defined in Eq.(25). We show in (1) that $F(0) > 0$, in (2) that $F(K) \rightarrow -\infty$ for $K \rightarrow \infty$ when $U/J < 36/\pi$ and in (3) that for $U/J < 36/\pi$ one has $F'(K) < 0$: one may then conclude that the equation $F(K) = 0$ has only one root for $U/J < 36/\pi$. Finally, we derive an analytic expression for $F(K)$ holding for small U/J .

From Eq.(25) one can see that:

(1) for $U/J \rightarrow 0$ one has $2 + \frac{\pi}{4} - \pi K = 0$, from which $K = \frac{8+\pi}{4\pi}$ and $K_B T_{BKT} \simeq 1.128J$: indeed, for small U/J , one has that

$$\frac{X_u K^2}{2} - \frac{n^2}{2} \log\left(1 + \frac{X_u K^2}{n^2}\right) = \frac{X_u K^2}{2} - \frac{n^2}{2} \left(\frac{X_u K^2}{n^2} - \frac{X_u^2 K^4}{2n^4} + \dots \right) = \frac{X_u^2 K^4}{4n^2} - \dots$$

and thus

$$\frac{1}{X_u K^2} g(K, X_u) \approx \frac{1}{X_u K^2} \sum_{n=1}^{\infty} \frac{X_u^2 K^4}{4n^2} \rightarrow 0.$$

In the same way, $F(K) \rightarrow 2 + \frac{\pi}{4}$ for $K \rightarrow 0$.

(2) $F(K) \rightarrow -\infty$ per $K \rightarrow \infty$ for $x_u < 3/2$ (where $x_u = \pi^2 X_u / 24 = \pi U / 24J$): indeed for large K

$$F(K) \approx 2 - \pi K \left(1 - \frac{1}{48x_u K^3} \int_0^{2\sqrt{6}\sqrt{x_u}K} dx x^2 \right) = 2 - \pi K \left(1 - \frac{\sqrt{6}}{3} \sqrt{x_u} \right) :$$

then, for $K \rightarrow \infty$, $F(K) \rightarrow -\infty$ with $x_u < 3/2$ and $F(K) \rightarrow \infty$ with $x_u > 3/2$.

(3) For $x_u < 3/2$, it is $F'(K) < 0$ for $K > 0$: indeed

$$F'(K) = -\pi - \frac{2\pi}{X_u K^3} g(K, X_u) + \frac{\pi^2 X_u^{1/2}}{2} \left[\coth(\pi X_u^{1/2} K) - \frac{1}{\pi X_u^{1/2} K} \right]. \quad (\text{A1})$$

Since $\lim_{x \rightarrow 0} \left(\coth x - \frac{1}{x} \right) = 0$, one gets

$$\lim_{K \rightarrow 0} F'(K) = -\pi.$$

For large K one finds

$$F'(K) \approx -\pi + \frac{\pi^2}{6} X_u^{1/2}.$$

Therefore one has that $\lim_{K \rightarrow \infty} F'(K) < 0$ for $X_u < 36/\pi^2$, and $\lim_{K \rightarrow \infty} F'(K) > 0$ for $X_u > 36/\pi^2$. Using similar arguments, one can show that, for $K > 0$, it is

$$F'(K) < -\pi + \frac{\pi^2}{6} X_u^{1/2}. \quad (\text{A2})$$

which implies that, for $X_u < 36/\pi^2$, one has $F'(K) < 0$. The behavior of $F(K)$ and $F'(K)$ for three values of U/J respectively smaller than, equal to and larger than $36/\pi$ is plotted in Figs. 2 and 3.

One may also obtain an analytic approximation for $F(K)$ holding for $U/J \ll 1$ by putting $z = \sqrt{X_u}K$ and using $\log(1+z) = \sum_{j=1}^{\infty} \frac{(-1)^{j+1} z^j}{j}$ for $|z| < 1$: one has

$$g(K, X_u) = \sum_{j=2}^{\infty} \frac{(-1)^j z^{2j}}{2j} \zeta(2j-2) \quad (\text{A3})$$

where $\zeta(j) = \sum_{n=1}^{\infty} \frac{1}{n^j}$ is the Riemann zeta-function. One finds

$$\sum_{j=2}^{\infty} \frac{(-1)^j z^{2j}}{2j} \zeta(2j) = \frac{1}{2} \left\{ \frac{\pi^2 z^2}{6} + \log \frac{\pi z}{\sinh \pi z} \right\}. \quad (\text{A4})$$

For large n one has the recurrence relation [27]

$$\zeta(n+1) \simeq \frac{1}{2}[1 + \zeta(n)].$$

Substituting back in Eq.(A3) and using (A4), one has

$$g(K, X_u) \approx X_u K^2 \left(\frac{\pi^2}{3} - \frac{3}{2} \right) + 2 \log \frac{\pi X_u^{1/2} K}{\sinh \pi X_u^{1/2} K} + \frac{3}{2} \log(1 + X_u K^2)$$

and finally

$$F \approx 2 - \pi K \left[1 - \frac{1}{4K} - \frac{1}{X_u K^3} \left(X_u K^2 \left(\frac{\pi^2}{3} - \frac{3}{2} \right) + 2 \log \frac{\pi X_u^{1/2} K}{\sinh \pi X_u^{1/2} K} + \frac{3}{2} \log(1 + X_u K^2) \right) \right]. \quad (\text{A5})$$

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FIGURES

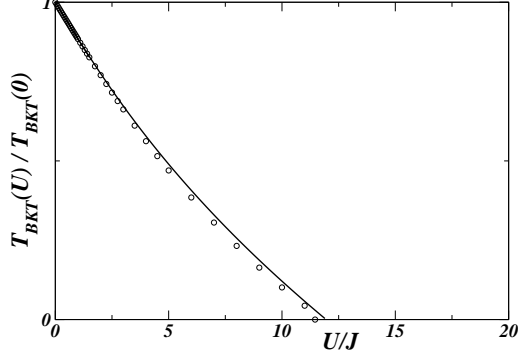


FIG. 1. The BKT critical temperature $T_{BKT}(U)$ (in units of $T_{BKT}(0)$) as a function of U/J . Empty circles: numerical solution of Eq.(25); solid line: Eq.(27).

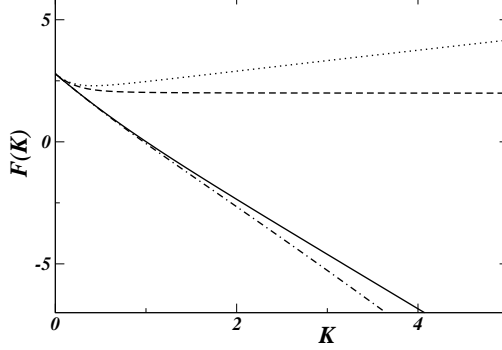


FIG. 2. $F(K)$ for $U/J = 1$ (solid line), $36/\pi$ (dashed line) and 15 (dotted line). The dot-dashed line is the analytic approximation (A5) for F holding for $U/J \ll 1$. For $U/J = 36/\pi$ F asymptotically tends to 0.

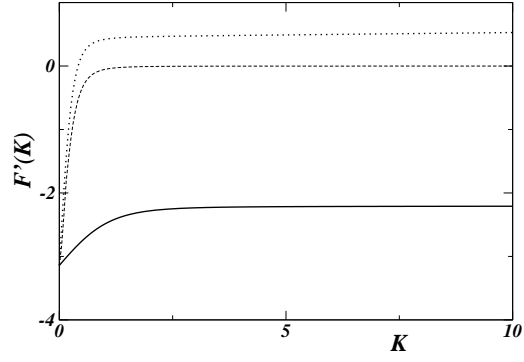


FIG. 3. $F'(K)$ for $U/J = 1$ (solid line), $36/\pi$ (dashed line) and 15 (dotted line).