Effect of zero-point fluctuations on the long-range phase coherence of granular films

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The quantum Hamiltonian $H = H_C + H_J$, with H_J the Josephson and H_C the charging energy between grains, is studied. Renormalization-group equations are derived within a semiclassical approximation that show that *there is a reentrant* normal phase for nonzero H_C; phase coherence is stable in a region of temperature that shrinks to zero as the quantum fluctuations grow, up to a critical value. The possible connection of these results to recent experiments is discussed.

Several years ago Abeles pointed out that the charging energy between grains could destroy the long-range phase coherence in granular materials.[1] Recently, several experiments have been carried out in granular films,[2] with the aim at testing the vortex-unbinding picture of Kosterlitz, Thouless, and Berezinskii (KTB)[3] to explain their resistive transition.[4] Recently different authors have incorporated the charging energy fluctuations into the KTB picture, most of them within a mean-field (MF) or a self-consistent-harmonic approximation.[5,6] Doniach, on the other hand, has estimated the effect of quantum fluctuations on the renormalized superfluid density by using a three-dimensional (3D) scaling argument.[7] It is known, however, that the detailed properties of the KTB transition itself cannot be predicted from a standard MF approach. In this Rapid Communication I present the results of a renormalization-group (RG) analysis of the effects of zero-point fluctuations (ZPF) on the KTB scenario, within a semiclassical approximation, i.e., in terms of an expansion in $\hbar$. I shall begin presenting the main results of this paper, then giving the highlights of the calculation, and at the end I will compare the results, where appropriate, with those of other authors as well as their possible connection to recent experimental results. Other results pertaining to this problem will be given elsewhere.[8]

A regular array of grains can be described by the Hamiltonian[5-7]

$$H = \frac{u}{2} \sum n_i^2 + \sum_i E_J [1 - \cos(\psi_{i+1} - \psi_i)] \quad . \tag{1}$$

The first term corresponds to the charging energy, whereas the second to the Josephson energy between grains. Here ψ_i is the phase difference of the superconducting order parameter between grains and n_i is the electron number operator that measures the deviation from the average number of electrons in the ith grain. The operators ψ_i and n_i are conjugate canonical variables,[1] i.e., $n_i = -i\partial/\partial\psi_i$; E_J is the Josephson coupling constant and $u = e^2/2C$, with C the average local capacitance between a pair of grains and e the electric charge.[9] The limit $u = 0$ corresponds to the classical KTB problem, whereas for $u \neq 0$ the quantum effects become relevant. To find the leading corrections to the classical limit I shall consider an expansion for u small. For u large the grains are small and localization effects become dominant.[10]

The results of this paper can be expressed in terms of the natural dimensionless parameter appearing in the theory

$$x = u/24E_J \quad . \tag{2}$$

The RG recursion formulas read

$$\frac{dK}{dl} = 4\pi^3 K^2 \tilde{y}^2 (1 - Kx)/(2Kx - 1) \quad , \tag{3a}$$

$$\frac{d\tilde{y}}{dl} = [2 - \pi K(1 - Kx)]\tilde{y} \quad , \tag{3b}$$

where $\tilde{y} \sim \exp[-(\pi^2/2)K(1 - Kx)]$ and $K = E_J/k_B T$, with k_B representing Boltzmann's constant and T the temperature. These equations are valid for $\tilde{y}$ small and reduce, as they should, to the Kosterlitz RG equations for $x = 0$.[3] The RG flow diagram resulting from Eq. (3) has two hyperbolic points ($\tilde{y} = 0$) at $K_2(x)$ and $K_{\rm KT}(x)$ and an elliptic point at $K_1(x)$. Also the line $K^{-1} = x$ represents an asymtote below of which the flow is unstable (see Fig. 1). From the solution to Eq. (3) I find that

$$K_{\rm KT}^{-1} = 2x/(1 - \sqrt{1 - 8x/\pi}) \quad . \tag{4}$$

The elliptic point is given by $K_1 = 1/2x$ and $K_2(x)$ by the same formula as Eq. (4) except that the sign before the radical is plus instead of minus. As x grows from zero the three especial points K_1, K_2, and $K_{\rm KT}$ approach each other until, *at the critical value*, $x_c = \pi/8$, they coalesce into one. Above x_c all the RG flow lines are unstable. Physically the

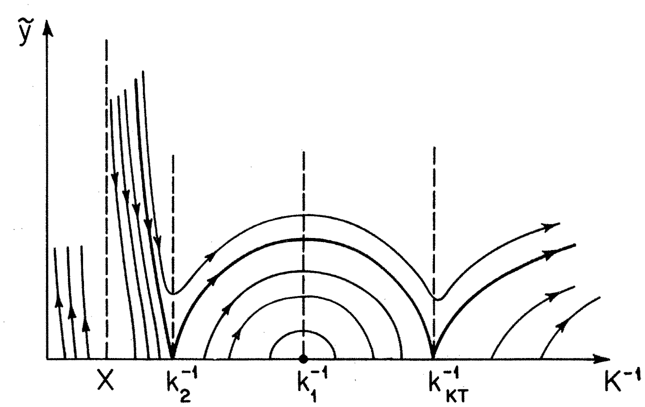

FIG. 1. Qualitative renormalization-group flow diagram resulting from Eq. (3). The quantities marked in the axis are defined in the text.

above results mean that as we increase the charging energy, i.e., when the grains decrease in size, the critical temperature decreases. At the same time, the phase coherent state is rendered unstable at lower temperature due to the quantum fluctuations of the phase that increase the vortex pairs density. As x grows the intermediate temperature range in which phase coherence is stable shrinks until it dissappears completely and only the normal phase is stable at all temperatures. Another consequence from Eq. (3) is that the exponent η remains universal at $K_{\rm KT}(x)$, i.e., $\eta[K_{\rm KT}(x)]=\frac{1}{4}$.

Before I discuss the possible consequences of these results to experiments I will present the logic that leads to Eq. (3).

The basic idea is to do an expansion in $\hbar$ around the classical KT solution. This procedure and, in fact, the general form of the answer was first discussed by Wigner in 1932.[11] Here I shall follow a more convenient route using Feynman's path integrals.[12] The quantum partition function related to Eq. (1) is $Z_Q=\mathrm{Tr}e^{-\beta H}$. Here the trace is understood in the usual quantum-mechanical sense. To calculate Z_Q we first go to the imaginary time representation and then in terms of sums over histories we have

$$Z_Q=\int_{\rm periodic} d[\psi(\tau)]\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar} L(\psi)d\tau\right] , \qquad (6)$$

with

$$L(\psi)=\sum_i\left[\frac{\hbar^2}{2u}\left(\frac{d\psi_i(\tau)}{d\tau}\right)^2 + E_J\{1-\cos[\psi_{i+1}(\tau)-\psi_i(\tau)]\}\right] .$$

The path integral is carried out over the classical fields $\psi_i(\tau)\in[-\pi,\pi]$ that satisfy the quantum-mechanical periodicity condition $\psi_i(\tau+\beta\hbar)=\psi_i(\tau)$ and $0\le\tau\le\beta\hbar$. It is easy to see that the classical planar model limit is recovered when $u=0$, and the extreme quantum limit corresponds to $u>>1$. An appropriate way to evaluate Eq. (5) is to use the variational principle calculation discussed by Feynman.[12] In the semiclassical or high-temperature limit the τ range is small. It is convenient to consider a Taylor expansion around the average field

$$\bar{\psi}_i=\frac{1}{\beta\hbar}\int_0^{\beta\hbar}\psi_i(\tau)d\tau .$$

This constraint is easily added to Eq. (5) by

$$Z_Q=\int_{\rm periodic} d[\psi(\tau)]\int d[\bar{\psi}]\delta[\psi-\bar{\psi}] \times\exp\left[-\frac{1}{\hbar}\int_0^{\beta\hbar}L(\psi)d\tau\right] .$$

Next, the exponential can be expanded around $\bar{\psi}_i$ giving as a result

$$Z_Q=(4\pi\beta u)^{-1/2}\int d[\bar{\psi}]\exp\left[-\beta H_J[\bar{\psi}]-\frac{\beta^2 u}{24}H_J''[\bar{\psi}]\right] +O(u^2) ,$$

in which primes mean derivatives with respect to the argument, and H_J is equal to H but with $u=0$. Because of the periodicity property of H_J we can immediately write the final answer for Z_Q to order $\hbar^2$:

$$Z_Q\cong(4\pi\beta u)^{-1/2} \times\int d[\bar{\psi}]\exp\left[-\sum_i K(1-Kx)\cos(\bar{\psi}_i-\bar{\psi}_{i+1})\right] . \qquad (7)$$

Here I have left out an irrelevant constant in the exponent. The partition function given in Eq. (7) is identical in form to that of the planar model including the fact that $\bar{\psi}\in[-\pi,\pi]$ except that the coupling constant has been renormalized by the charging energy term in an important way. It is now easy to find the corresponding RG recursion formulas and then study their consquences. The resulting equations are those given in Eq. (3) and their implications were discussed above. These results have been obtained from considering the lowest-order correction due to the ZPF. The decrease of $T_{\rm KT}(x)$ should remain valid after including higher-order corrections in Z_Q. However, the reentrance phenomena could be an artifact of the lowest-order correction. The next nontrivial correction is of order $\hbar^4$. The four-loop calculation of Z_Q has essentially been done by Wigner as well.[11,12] In our case it gives

$$Z_Q^{(4)}=(4\pi\beta u)^{-1/2}\int d[\bar{\psi}]\,e^{-\beta H_J}\left[\frac{7}{10}K^4x^2H_J'^2-\frac{K^3x^2}{2}H_J\right] , \qquad (8)$$

where I used explicitly the fact that H_J is periodic. If we were to add to the exponential the last term, the RG equation would be such that the reentrant temperature would be lower and thus one would surmise that the higher-order loops would kill the reentrance. However, the last two terms are of the same order and they cannot be simply added to the exponential. Because the reentrance occurs at low temperatures and the averages in Eq. (8) are taken with respect to the *classical* planar model, we can use known spin-wave results to estimate $Z_Q^{(4)}$. From a straightforward analysis I find that the spin-wave perturbation analysis breaks down when $Kx\approx 1$, signaling that an instability seems to exist at low temperatures to this order as well, and that $Z_Q^{(4)}\sim +(Kx)^2$. The sign here is all important to guarantee reentrance. Notice that $Kx\sim u/k_BT$ gives a measure of the relevance of the charging energy with respect to thermal fluctuations. This perturbative analysis gives further credence to the fact that a reentrant transition exists in this model within the semiclassical approximation up to four loops.[13] As Doniach has pointed out, at $T=0$ exactly, the model should behave more like a 3D x-y model and it should present its critical properties. However, the crossover from the quasi 2D model considered here to the 3D behavior cannot be ascertained by a semiclassical analysis alone.

In the experiment by Hebard and Vanderberg[2] it was found that the decrease of $T_{\rm KT}$ as a function of normal-sheet resistance, was much faster than the prediction from the classical[4] KT theory analysis. Simanek has suggested that the decrease should be due to charging energy effects.[14] He studied the model given in Eq. (1) within a MF and a self-consistent-harmonic approximation calculation that shows that $T_{\rm KT}$ does decrease as x increases. The decrease was found to be exponential in x and apparently closer to the experiment. The decrease found from Eq. (4) is, however, *much slower*. Hebard,[15] on the other hand, noticed that when the normal-sheet resistance is of the order of 10 to 30 kΩ, the resistance measured in his films instead of going to zero, flattened and possibly could increase at lower temperatures. This reentrant-type behavior has been seen by Kobayashi, Tada, and Sasaki, in granulated Sn films.[16] Both Hebar and Kobayashi *et al.* argued for a reentrant-type explanation to understand their experimental results. Simanek has noticed that because the resistance becomes flat without reaching zero, a percolative model would be more appropriate.[17] The generality of this suggestion has been questioned, however, by Kobayashi *et al.*[18] Here I have found what seems to be evidence that the model given by Eq. (1) has a reentrant transiton in the semiclassical limit. The special nature of the RG flows in the figure could conceivably accommodate the almost zero resistance state corresponding to a flow line that tends to the $\tilde{y}=0$ line but does not quite reach it. Although a realistic model for granular materials is hard to study, it seems that the qualitative trends of the quantities measured experimentally seem to follow the trends of the results found here.

In conclusion, I have studied for the first time the effect of zero-point fluctuations in the KTB scenario within a semiclassical approximation and RG analysis. The RG flows indicate the existence of a reentrant transition as well as a decrease of $T_{\rm KT}$ with x. Although a four-loop contribution was analyzed at low temperatures, nonperturbative studies are needed to ascertain *conclusively* the existence of the reentrant transition in this model.

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