Soluble supersymmetric quantum XY model

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We present a supersymmetric modification of the d-dimensional quantum rotor model whose ground state is exactly soluble. The model undergoes a vortex-binding transition from insulator to metal as the rotor coupling is varied. The Hamiltonian contains three-site terms which are relevant: they change the universality class of the transition from that of the $(d+1)$- to the d-dimensional classical XY model. The metallic phase has algebraic off-diagonal long-range order but the superfluid density is identically zero. Variational wave functions for single-particle and collective excitations are presented.

This paper discusses an exactly soluble modified version of the quantum XY model

$$\mathcal{H}_0 = -U\sum_j \frac{\partial^2}{\partial\theta_j^2} - J\sum_{j\delta}\cos(\theta_j - \theta_{j+\delta}), \tag{1}$$

where j is summed on sites of a hypercubic lattice and δ is summed on near-neighbor vectors.[1] This model is often used to describe the superconductor-insulator transition in granular superconductors and Josephson junction arrays.[2] The coupling constant J represents the strength of the Josephson coupling between the order parameter phases θ_i and θ_j on neighboring grains. The parameter U represents the charging energy of the grains. The boson (Cooper pair) number operator conjugate to the phase is the angular momentum $\hat{n}_j \equiv -i\partial_{\theta_j}$. While this is correctly quantized in integer values, it can be negative. Thus the model implicitly assumes a large background number n_0 of bosons per lattice site so that $\hat{n}_j$ represents local deviations (positive or negative) from this mean (integer) value. We can view the cosine term as a mutual torque which transfers quanta of angular momentum (bosons) from one site to the next. Thus the quantum XY model is essentially equivalent to (i.e., in the same universality class as) the boson Hubbard model. For large U/J the ground state is a Mott-Hubbard insulator and for small U/J it is superfluid which exhibits off-diagonal long range order (ODLRO) in the phase field correlations (at zero temperature)

$$G_{ij} \equiv \langle e^{i\theta_i} e^{-i\theta_j}\rangle \tag{2}$$

for dimension $d > 1$ (and algebraic ODLRO for $d = 1$). The transition between the superfluid and Mott-Hubbard insulating states is continuous and is in the universality class of the $d+1$-dimensional *classical* XY model.[2–4] The extra dimension arises from the fact that in the path integral representation of the partition function, the Euclidean time interval $0 \le \tau \le \hbar\beta$ diverges at zero temperature.

While the physics of this model is now completely understood, it has resisted exact solution in all dimensions. It is interesting to consider a Jastrow-like variational wave function

$$\psi_0(\theta_1,\ldots,\theta_N) = \exp\left[-\left(\frac{\lambda}{U}\right)V(\theta_1,\ldots,\theta_N)\right] \tag{3}$$

where λ is a variational parameter and

$$V \equiv -J\sum_{j\delta}\cos(\theta_j - \theta_{j+\delta}) \tag{4}$$

is the potential energy from Eq. (1). This form is motivated by the harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 \tag{5}$$

for which the exact ground state is

$$\psi(x) = \exp\left[-\hbar\omega\left(\frac{1}{2}Kx^2\right)\right]. \tag{6}$$

The variational state in Eq. (3) is thus in the spirit of the harmonic spin-wave approximation in which one expands the cosine term to second order in deviations from the classical ground state. The wave function is much better than this however because it obeys the correct periodicity under $\theta_j \to \theta_j + 2\pi$. This feature is crucial to the existence of (quantum) vortices in the ground state and hence allows for the possibility of a phase transition to the insulating state physics which is completely missing from the spin-wave approximation.

The purpose of the present paper is to examine the variational wave function of Eq. (3) and to consider a Hamiltonian for which ψ_0 happens to be the exact ground state.[5] The question of what Hamiltonians have Jastrow wave functions for ground states has a long history[6,7] and this question has recently been reexamined from a modern perspective by Kane *et al.*[8] Except for special cases,[7] the generic requirement is that the Hamiltonian have three-body interactions of a particular form. We will see shortly that the analog of this for the present problem is three-site interactions. Kane *et al.* argue that these three-body interactions are (perturbatively) irrelevant in the renormalization-group sense. That is, they have no effect on the long-distance properties of the system (other than a trivial renormalization of the

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speed of sound). This result is perturbative because it neglects vortexlike excitations.[8] While, strictly speaking, the above statements are true, they can be quite misleading if the ground state of the system undergoes a phase transition. We show explicitly below that the universality class of the transition is completely altered by the inclusion of particular three-site interactions. This is a nonperturbative effect precisely due to the role played by vortices in the (zero temperature) transition. The discussion below in readily generalized to any dimension, but for definiteness we consider only the case $d = 2$.

We construct the desired Hamiltonian by defining the operators

$$Q_j = \sqrt{U}\frac{\partial}{\partial\theta_j} + \frac{J}{\sqrt{U}}\sum_\delta\left[\sin(\theta_j - \theta_{j+\delta}) + \sin(\theta_j - \theta_{j-\delta})\right], \tag{7a}$$

$$Q_j^\dagger = -\sqrt{U}\frac{\partial}{\partial\theta_j} + \frac{J}{\sqrt{U}}\sum_\delta\left[\sin(\theta_j - \theta_{j+\delta}) + \sin(\theta_j - \theta_{j-\delta})\right]. \tag{7b}$$

It is readily verified using Eq. (3) that

$$Q_j\psi_0 = 0 \tag{8}$$

for every j (we take $\lambda = 1$ hereafter).

The supersymmetric[9,5] Hamiltonian

$$H = \sum_j Q_j^\dagger Q_j \tag{9}$$

is clearly positive semidefinite and therefore ψ_0 is an exact, zero-energy ground state of H. Using Eq. (7a) we can write H in the form

$$H = -U\sum_j \partial_{\theta_j}^2 - J\sum_{j\delta}\cos(\theta_j - \theta_{j+\delta}) + \frac{J^2}{U}\sum_{j\delta\delta'}\sin(\theta_j - \theta_{j+\delta})\sin(\theta_j - \theta_{j+\delta'}). \tag{10}$$

The first two terms on the right-hand side are equivalent to the usual quantum XY model of Eq. (1). The remaining term is a perturbation consisting of two- and three-site interactions. These terms represent the simultaneous hopping of a pair of bosons. The $\delta = \delta'$ terms give rise to a $\cos 2\theta$ coupling, a form which has been studied by Lee and Grinstein.[10]

Now that we have the Hamiltonian and the exact ground state, let us examine the nature of the ground state as a function of the quantum fluctuation parameter U/J to see if the system undergoes a phase transition. The (unnormalized) probability distribution of the phase angles is

$$P[\theta_1, \theta_2, \ldots, \theta_N] \equiv |\psi_0|^2 = \exp\left\{\frac{2J}{U}\sum_{j\delta}\cos(\theta_j - \theta_{j+\delta})\right\} \tag{11}$$

which is identical to the Boltzmann factor for the *classical* two-dimensional (2D) XY model with $U/2J$ playing the role of dimensionless temperature. This model undergoes a Kosterlitz-Thouless phase transition at a critical temperature[11] $U/2J \approx 0.9$. This is clearly a different universality class from that of the usual 2D quantum XY model which is known to be in the universality class of the 3D XY model. Thus we see that the three site terms are relevant to the transition [at least when they have the particular strength given in Eq. (10)].

If we knew the exact ground state $\Phi(\theta_1, \ldots, \theta_N)$ of the usual quantum rotor problem, then $|\Phi|^2$ would of course define a 2D classical statistical mechanics problem. However, the fake classical Hamiltonian would necessarily contain long-range forces (in order to give the 3D XY universality class in a 2D model[5]).

We are used to the notion that thermal fluctuations produce vortices. Here we see a nice illustration of the fact that even at zero temperature, vortices can be produced by quantum fluctuations. For $U/2J > T^*_{\rm KT}$ the largest amplitude configurations in the ground state contain free vortices and the spin-spin correlation function decays exponentially

$$G_{ij} \equiv \langle e^{i\theta_i}e^{-i\theta_j}\rangle \sim e^{-|\mathbf{R}_i - \mathbf{R}_j|/\xi}, \tag{12}$$

whereas for $U/2J < T^*_{\rm KT}$ the correlations decay only algebraically

$$G_{ij} \sim |\mathbf{R}_i - \mathbf{R}_j|^{-\eta} \tag{13}$$

because vortices are confined. That is, virtual vortex-antivortex "vacuum fluctuations" appear but do not proliferate.

Knowing the ground state exactly, we use Feynman's theory for superfluid ^{4}He to motivate variational excited state wave functions. In a Bose system the excited state wave function has to be symmetric under exchange of two particles, and must have a node to be orthogonal to the ground state. From these two arguments, Feynman has shown that the only low-lying excited states of a Bose system are the long wavelength collective density waves. We want to write an excited state wave function which preserves the short-range correlations of the ground state but is orthogonal to it. The following Feynman-Bijl–type[12] wave function, which is a product of the ground-state wave function and another symmetric function $\rho_{\mathbf{q}}$, satisfies this condition

$$\Psi_{\mathbf{q}} = \rho_{\mathbf{q}}\Psi_0. \tag{14}$$

As discussed below, the form of $\rho_{\mathbf{q}}$ depends on the choice of excitation. If the excited state is orthogonal to the ground state, i.e.,

$$\langle\Psi_{\mathbf{q}}|\Psi_0\rangle = 0 \tag{15}$$

then we can use the variational principle to find an upper bound on the excitation energy (taking advantage of the fact that the ground-state energy vanishes)

$$\Delta_{\mathbf{q}} \le \frac{\langle\Psi_{\mathbf{q}}|H|\Psi_{\mathbf{q}}\rangle}{\langle\Psi_{\mathbf{q}}|\Psi_{\mathbf{q}}\rangle} \tag{16}$$

where $\langle\Psi_{\mathbf{q}}|H|\Psi_{\mathbf{q}}\rangle = f(\mathbf{q})$ is the oscillator strength, and $\langle\Psi_q|\Psi_q\rangle = s(\mathbf{q})$ is the static structure factor. Writing $\Psi_{\mathbf{q}}$ is terms of Ψ_0:

$$\begin{aligned} f(\mathbf{q}) &= \langle\Psi_{\mathbf{q}}|H|\Psi_{\mathbf{q}}\rangle \\ &= \langle\Psi_0|\rho_{-\mathbf{q}}H\rho_{\mathbf{q}}|\Psi_0\rangle, \end{aligned} \tag{17}$$

and writing the Hamiltonian in terms of Q's and using the fact that $Q_j\Psi_0 = 0$,

$$f(\mathbf{q}) = \langle\Psi_0|[\rho_{-\mathbf{q}}, Q_j^\dagger][Q_j, \rho_{\mathbf{q}}]|\Psi_0\rangle \tag{18}$$

By substituting an explicit form of $\rho_{\mathbf{q}}$ in the above results, $f(\mathbf{q})$ can be calculated immediately.

First we consider an excited-state wave function which describes a single-particle excitation:

$$\Psi_{\mathbf{q}} = b_q^\dagger\Psi_0 \tag{19}$$

where

$$b_{\mathbf{q}}^\dagger = \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{q}\cdot\mathbf{R}_j}e^{i\theta_j} \tag{20}$$

is the spatial Fourier transform of the operator that adds a unit of angular momentum at site j. Using Eq. (20)

$$[Q_j, b_{\mathbf{q}}] = \sqrt{U/N}e^{i\mathbf{q}\cdot\mathbf{R}_j}e^{i\theta_j} \tag{21}$$

it follows that $f_{\mathbf{q}} = \langle\Psi_0|b_{-\mathbf{q}}Hb_{\mathbf{q}}|\Psi_0\rangle = U$. The static structure factor is given by the spin susceptibility of the classical XY model at wave vector $\mathbf{q}$

$$s(\mathbf{q}) = \frac{1}{N}\sum_{ij} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle\Psi_0|e^{i(\theta_i-\theta_j)}|\Psi_0\rangle \tag{22}$$

which we know from Kosterlitz-Thouless theory:

$$\langle e^{i\theta_i}e^{-i\theta_j}\rangle \sim \begin{matrix} |\mathbf{R}_i-\mathbf{R}_j|^{-\eta}, & T<T_c, \\ e^{-|\mathbf{R}_i-\mathbf{R}_j|/\xi}, & T>T_c, \end{matrix} \tag{23}$$

where T_c is the critical temperature, or critical coupling $(U/J)_c$ in our case, with η ranging from 0 to $\frac{1}{4}$ as temperature varies from 0 to T_c. In the spin-wave approximation $\eta = \frac{U}{4\pi J}$ for our model. Substituting Eq. (23) in Eq. (22), and changing summations to integrals for an infinitely large system with U/J below the critical point

$$s(\mathbf{q}) \sim \frac{1}{2\pi}\int_0^\infty r^{-\eta+1}J_0(qr)dr \sim q^{-2+\eta}, \tag{24}$$

where $r = |\mathbf{R}_i - \mathbf{R}_j|$ and since $f(\mathbf{q}) = U$

$$\Delta(\mathbf{q}) \sim \frac{U}{s(\mathbf{q})} \sim Uq^{2-\eta}. \tag{25}$$

For U/J above the critical point and $q\xi \ll 1$

$$s(\mathbf{q}) = \frac{1}{2\pi}\int_0^\infty drre^{-r/\xi}J_0(qr) \sim \xi^2 \tag{26}$$

and hence the quantum system has an excitation gap (within the single mode approximation)

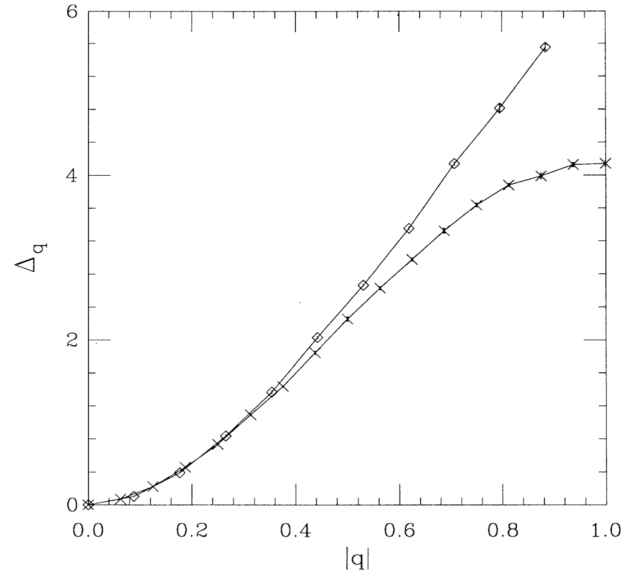

FIG. 1. Excitation energy $\Delta_{\mathbf{q}}$ as a function of $\mathbf{q}$ for $U/J = 0.8$ and 0.9. The (×) are for $\mathbf{q}$ in the (1,0) direction and the (◇) are for $\mathbf{q}$ in the (1,1) direction. For small $\mathbf{q}$, the single-particle model is isotropic.

$$\Delta(\mathbf{q}=\mathbf{0}) \sim U\xi^{-2}. \tag{27}$$

Using the Kosterlitz-Thouless (KT) theory[13] prediction for the correlation length we have

$$\Delta(0) \sim \exp\left\{-2b\left[\frac{J}{U} - \left(\frac{J}{U}\right)_c\right]^{-1/2}\right\} \tag{28}$$

where b is a positive constant.

Figures (1) and (2) illustrate the basic features of the

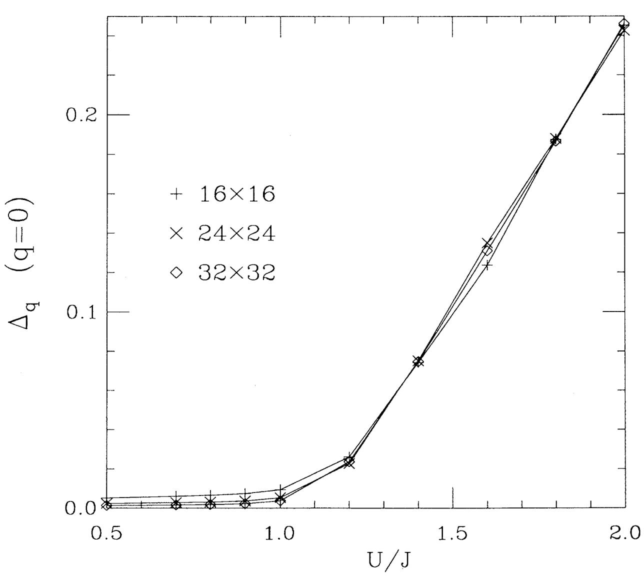

FIG. 2. Single-particle excitation energy vs coupling at $\mathbf{q} = 0$, for different system sizes. Notice that $\Delta_{\mathbf{q}} \to 0$ as the system size increases for U/J below the critical point.

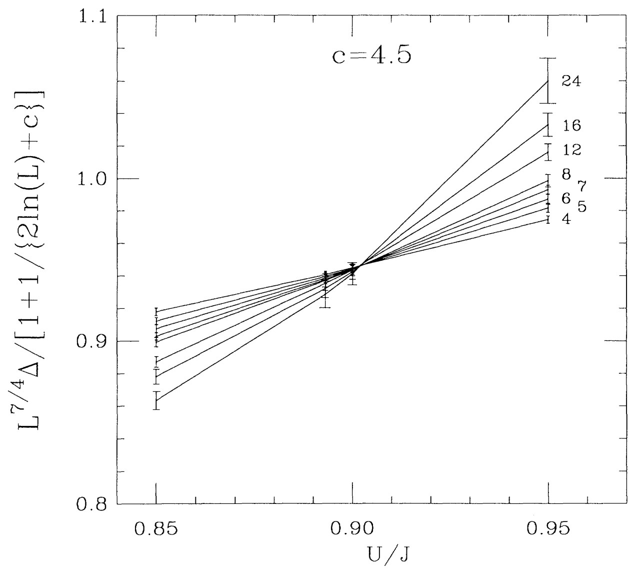

FIG. 3. Estimation of critical coupling for the single-particle model. $L^{7/4}\Delta(\mathbf{0})$ is independent of system size L at the critical point according to the Kosterlitz-Thouless theory. The logarithmic factor is a correction to scaling (see text). The parameter $C \sim 4.5$ was adjusted to obtain the best scaling.

excitation energy. In the thermodynamic limit the system is gapless below the critical point and has a gap which rises from zero above the critical point with the essential singularity characteristic of the KT transition. In the ordinary quantum XY model, the Bogoliubov process mixes the single-particle and density excitations to produce a linearly dispersing collective Goldstone mode in contrast to the $\omega \sim q^2$ dispersion of free bosons. We see here from Eq. (25) a curious contrast to the generic behavior. The collective mode dispersion $\omega \sim q^{2-\eta}$ gradually stiffens with increasing U/J but never becomes linear since $\eta \leq 1/4$ below the transition. We note that since we have only a variational excited state, our excited state energy is only an upper bound to the true energy. However, this does not affect our conclusion that the mode dispersion is softer than linear. It is at least as soft as $\omega \sim q^{2-\eta}$.

Notice that right at the critical point the $q = 0$ single-particle energy only vanishes in the thermodynamic limit $L \to \infty$ since the classical XY model susceptibility obeys $s(\mathbf{q}) \sim \int d^2r\ r^{-1/4} \sim L^{7/4}$. Thus we expect $L^{7/4}\Delta(\mathbf{0})$ to be scale-invariant (i.e., independent of L) at the critical point, provided L is large enough. Using data from lattices with $8 \leq L \leq 24$ we found the scale-invariant point to be $U/J \sim 0.905$. On general renormalization-group grounds we expect logarithmic corrections to scaling for small L in the 2D XY model.[11] We include these corrections in Fig. 3 where we plot $L^{7/4}\Delta(\mathbf{0})/[1+1/(2\ln L+4.5)]$ vs U/J. We again find the critical value $U/J \sim 0.905$ but the scaling now works well all the way down to $L = 4$. Our value for the critical coupling is close to, but somewhat above, the value of $U/J \sim 0.895$ found by Olsson and Minnhagen[11] using the scaling of the superfluid density.

We turn now to a study of the collective density mode excited state by taking $\rho_{\mathbf{q}}$ to be the Fourier transform of the number density

$$\rho_{\mathbf{q}} = \sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i}(-i\partial_{\theta_i}) \tag{29}$$

so that

$$\Psi_{\mathbf{q}} = \frac{iJ}{U}\sum_{i\delta} e^{i\mathbf{q}\cdot\mathbf{R}_i}\ \{\sin(\theta_i - \theta_{i+\delta}) + \sin(\theta_i - \theta_{i-\delta})\}\Psi_0. \tag{30}$$

The static structure factor is

$$s(\mathbf{q}) = \frac{J^2}{U^2}\sum_{ij\delta\delta'} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\ \langle\Psi_0|\ [\sin(\theta_i - \theta_{i+\delta}) + \sin(\theta_i - \theta_{i-\delta})][\sin(\theta_j - \theta_{j+\delta'}) + \sin(\theta_j - \theta_{j-\delta'})]|\Psi_0\rangle. \tag{31}$$

Following the steps in the calculation of oscillator strength for the single-particle model, we find $f(\mathbf{q})$ for the density-wave state to be

$$\begin{aligned} f(\mathbf{q}) = \langle\Psi_0|\frac{J^2}{U}\sum_{j\delta\delta'}\{&(1-e^{i\mathbf{q}\cdot\boldsymbol{\delta}})(1-e^{-i\mathbf{q}\cdot\boldsymbol{\delta}'})\cos(\theta_j-\theta_{j+\delta})\cos(\theta_j-\theta_{j+\delta'}) + (1-e^{-i\mathbf{q}\cdot\boldsymbol{\delta}})(1-e^{-i\mathbf{q}\cdot\boldsymbol{\delta}'}) \\ &\times\cos(\theta_j-\theta_{j-\delta})\cos(\theta_j-\theta_{j+\delta'}) + (1-e^{i\mathbf{q}\cdot\boldsymbol{\delta}})(1-e^{i\mathbf{q}\cdot\boldsymbol{\delta}'})\cos(\theta_j-\theta_{j+\delta})\cos(\theta_j-\theta_{j-\delta'}) \\ &+(1-e^{-i\mathbf{q}\cdot\boldsymbol{\delta}})(1-e^{i\mathbf{q}\cdot\boldsymbol{\delta}'})\cos(\theta_j-\theta_{j-\delta})\cos(\theta_j-\theta_{j-\delta'})\}|\Psi_0\rangle. \end{aligned} \tag{32}$$

We performed Monte Carlo simulations of the 2D XY model to find the excited-state energy $\epsilon_{\mathbf{q}} \leq f(\mathbf{q})/s(\mathbf{q})$ for systems of finite size. Though one expects some physical connection between single-particle and density-mode approximations, our results for the two excitations are quite different. We found that unlike single-particle excitation, the density wave is gapped and nearly dispersionless. Consequently, the results do not change significantly with the system size in the latter case. The excited-state energy $\epsilon_{\mathbf{q}}$ vs $\mathbf{q}$ is shown in Fig. 4, with $\mathbf{q}$ in (1,0) direc-

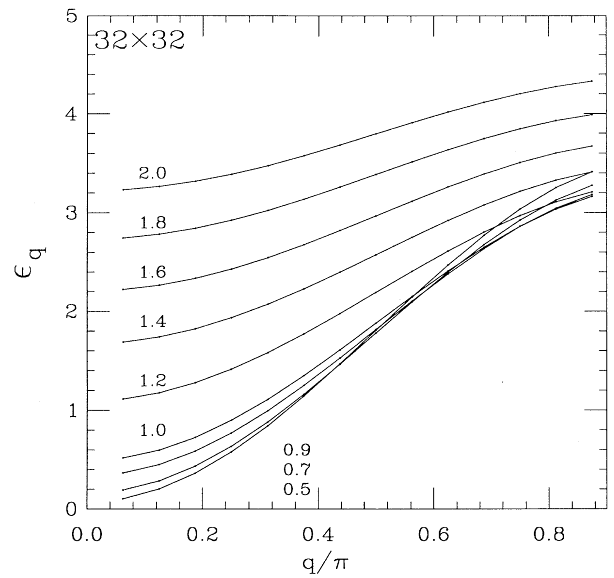

FIG. 4. Excitation energy $\epsilon_{\mathbf{q}}$ vs. $\mathbf{q}$ for single-mode density-wave approximation. $\mathbf{q}$ is in the (1,0) direction. The value of the coupling U/J is shown next to each curve.

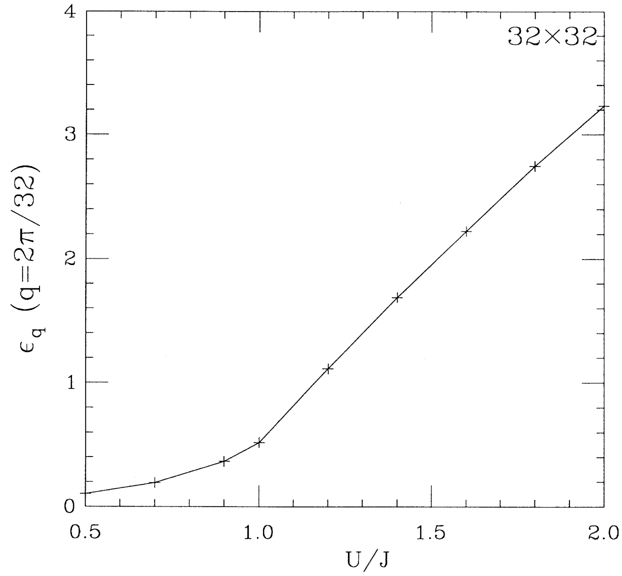

FIG. 5. The density-wave excitation energy $\epsilon_{\mathbf{q}}$ increases gradually as a function of U/J in the single-mode approximation. The results are for $\mathbf{q} = (\frac{2\pi}{32}, 0)$, the smallest nonzero allowed wave vector on a 32×32 lattice.

tion. Figure 5 is a plot of $\epsilon_{\mathbf{q}}$ vs U/J for the smallest nonzero allowed vector on a 32×32 lattice, i.e., $(\frac{2\pi}{32}, 0)$. We notice that the excited-state energy for this model increases gradually with coupling U/J, contrary to the single-particle case, where the energy is close to zero below the critical point, and then abruptly increases. We do not have independent evidence for the accuracy of our variational excited states. We must therefore interpret the collective gap as simply an upper bound to the exciation energy. We again emphasize however that our variational results for the very soft single-particle mode rigorously prove that the generic Bagoliubov process fails to occur for this model.

We conclude with some comments on additional curious features of this model. The model is readily extended to include exact solutions for arbitrary random bond strengths $J_{i,\delta}$ and frustration vector potential $A_{i,\delta}$. One might imagine that since the ground-state energy is identically zero independent of the disorder realization, one could compute ensemble-averaged correlation functions without having to invoke the replica trick.[14] This is not possible however since the *norm* of the ground wave function

$$\Phi(\theta_1, \ldots, \theta_N) = \exp\left\{\sum_{j\delta} \frac{J_{j,\delta}}{U} \cos\left(\theta_j - \theta_{j+\delta} + A_{j\delta}\right)\right\} \tag{33}$$

does depend on the disorder. A second consequence of the ground-state energy being zero for all $A_{j,\delta}$ is that *the superfluid density is identically zero* at $T = 0$ *even though the system exhibits (algebraic) ODLRO below the critical value of* U/J.

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