Superfluid to Mott-Insulator Transition in Bose-Hubbard Models

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We study the superfluid-insulator transition in Bose-Hubbard models in one-, two-, and three-dimensional cubic lattices by means of a recently proposed variational wave function. In one dimension, the variational results agree with the expected Berezinskii-Kosterlitz-Thouless scenario of the interaction-driven Mott transition. In two and three dimensions, we find evidence that, across the transition, most of the spectral weight is concentrated at high energies, suggestive of preformed Mott-Hubbard sidebands. This result is compatible with the experimental data by Stoferle *et al.* [Phys. Rev. Lett. **92**, 130403 (2004)].

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Recent experiments on cold atoms trapped in optical lattices demonstrated that the Mott transition (MIT), originally introduced in electronic systems [1], can be experimentally realized also in bosonic systems [2], where the MIT is actually a superfluid-insulator transition. Recent experiments by Stoferle *et al.* [3] have shown that a considerable amount of spectral weight is concentrated at high energy even within the superfluid phase. More specifically, the data suggest that, especially in three dimensions, a Mott-Hubbard gap of order U (the strength of the intrawell repulsion) develops already on the superfluid side of the MIT, akin to what is predicted to occur in electronic systems [4]. Although this evidence is not incompatible with the accepted theory of the critical behavior across the superfluid-to-insulator transition [5], it clearly demands a more detailed comprehension that must also include high-energy excitations. There have been already several theoretical attempts, mainly based on suitable extensions of mean-field theory, to uncover the whole dynamical behavior across the MIT [6,7]. These calculations predict in the most general cases the existence of high-energy modes even in the superfluid phase that might explain the experimental data. However, when the transition is approached at fixed integer filling by tuning for instance the interaction strength, these theories also predict that all modes soften at the transition. In this work, we address this question by an alternative approach based on a variational wave function that has been recently proposed in the context of the electronic MIT [8–10]. The accuracy of the wave function is checked by comparison with Green's Function Monte Carlo (GFMC) simulations, that allow us to obtain numerically exact results by a stochastic sampling of the ground-state wave function [11]. In contrast with the aforementioned mean-field theories, we find that, at fixed density, the MIT is accompanied by a gradual transfer of spectral weight from the low-energy sound mode towards high energies, so that, when the Mott insulating phase is established, most of the spectral weight is already concentrated at high energy. In addition, our analysis uncovers features of variational wave functions able to describe a Mott transition that are novel and might be common to bosonic as well as fermionic systems.

Bosons trapped in optical lattices can be modeled by the Hubbard Hamiltonian [5,12–14]

$$\mathcal{H} = -\sum_{ij}(t_{ij}a_i^\dagger a_j + \text{H.c.}) + \frac{U}{2}\sum_i n_i(n_i - 1), \qquad (1)$$

where $a_i^\dagger$ (a_i) creates (annihilates) a particle at site i and $n_i = a_i^\dagger a_i$; t_{ij} is the hopping amplitude and U is the on-site repulsion. Experimentally, the ratio t_{ij}/U can be varied by changing the laser intensity [2,12,15], namely, the amplitude of the periodic potential which modifies both the interwell tunneling amplitude t_{ij} and the strength of the repulsive interaction U within a single potential well. The Hubbard model (1) at integer filling has generally two different phases: one superfluid, for $U < U_c$, and the other insulating, above U_c.

Our purpose in this Letter is to describe the MIT by means of a variational wave function. In spite of the fact that the variational approach is a simple and well established technique, its application to the MIT is extremely difficult. For instance, the celebrated Gutzwiller wave function is not appropriate to describe the MIT, as it leads to an unrealistic insulator with no density fluctuations [16,17]. Recently, an extension of the Gutzwiller wave function has been proposed [8], that proved to be very accurate to describe an electronic MIT in one dimension [8,10]. Here we apply the same variational approach to the Bose-Hubbard model (1) with nearest-neighbor hopping $t/2$ in a one-dimensional chain (1D), a two-dimensional (2D) square lattice, and a three-dimensional (3D) cubic lattice with L sites and periodic boundary conditions. We consider the following ansatz for the variational wave function

$$|\Psi\rangle = \exp\left(-\frac{1}{2}\sum_{i,j} v_{i,j} n_i n_j + g_{\mathrm{MB}} \sum_i \xi_i\right)|\Phi_0\rangle, \quad (2)$$

where $|\Phi_0\rangle$ is the noninteracting fully-condensed wave function, i.e., $|\Phi_0\rangle = (b^\dagger_{k=0})^N|0\rangle$, being $b^\dagger_k$ the creation operator at momentum k and $N = L$ the number of particles. The components of the Jastrow potential, $v_{i,j} = v(|R_i - R_j|)$, are independently optimized by a variational Monte Carlo (VMC) minimization of the total energy [18]. In the following, we will denote by ρ_q and v_q the Fourier transforms of the boson-density n_i and of the Jastrow parameters $v_{i,j}$, respectively. Finally, g_{MB} is a variational parameter related to the many-body operator $\xi_i = h_i \prod_\delta (1 - d_{i+\delta}) + d_i \prod_\delta (1 - h_{i+\delta})$, where $h_i = 1$ ($d_i = 1$) if the site i is empty (doubly occupied) and 0 otherwise, and δ is the vector that connects nearest-neighbor sites [19]. This term is kept just to improve the variational accuracy (mainly in two dimensions and three dimensions) but does not introduce important correlation effects, that are instead contained only in the *long-range* tail of the two-body Jastrow potential $v_{i,j}$.

Although our ultimate scope is to uncover some dynamical properties across the MIT, we think it is worth discussing in some detail the role of the Jastrow factor in (2), which is the novel ingredient with respect to the conventional Gutzwiller wave function. In the superfluid phase, a long-range Jastrow potential is needed to restore the correct small-q behavior of the static density structure factor [13], i.e., $N_q = \langle\Psi|\rho_{-q}\rho_q|\Psi\rangle/\langle\Psi|\Psi\rangle \sim |q|$. Indeed, since at least at weak coupling, the expression

$$N_q = \frac{N_q^0}{1 + \gamma v_q N_q^0} \quad (3)$$

holds with $\gamma = 2$, [20] and because the noninteracting $N_q^0 = \langle\Phi_0|\rho_{-q}\rho_q|\Phi_0\rangle \sim \text{const}$, it follows that $v_q \sim 1/|q|$. Assuming that the expression (3) remains valid for $|q| \to 0$ even in the Mott insulating phase, one might be tempted to believe that $v_q \sim 1/q^2$ is necessary and sufficient to recover in any dimension the appropriate $N_q \sim q^2$ insulating behavior, consequence of exponentially decaying correlation functions. However, one easily realizes that, were this conclusion correct, the variational wave function (2) could not describe any bosonic insulator in 3D, since $v_q \sim 1/q^2$ is not sufficient to empty the condensate fraction. [21] Indeed, as shown below, the optimized variational wave function has a more diverging $v_q \sim 1/|q|^3$ in the 3D Mott insulator, although $N_q \sim q^2$, implying that the formula (3) does not generally hold.

In Fig. 1 we draw the optimized Jastrow potential v_q. For any dimension, the MIT is clearly signaled by the sudden change in the small-q behavior of v_q. On the one hand, the superfluid phase is always described by $v_q \sim \alpha/|q|$, with α increasing with U. On the other hand, the Mott insulator has a much more diverging v_q. In one dimension we recover the $v_q \sim 1/q^2$ behavior, like in the fermionic case. [8] In two dimensions, the leading behavior of the Jastrow potential across the transition is less clear-cut than in one dimension. Indeed, we cannot establish whether, on the insulating side, the leading behavior is given by $v_q \sim \beta_{2\mathrm{D}}/q^2$ with $\beta_{2\mathrm{D}}$ large but finite, or logarithmic corrections have to be considered, i.e., $v_q \sim \ln(1/|q|)/q^2$. Finally, in three dimensions a more diverging $v_q \sim 1/|q|^3$ is stabilized in the insulating regime. Therefore, in all cases the Jastrow potential is able to empty the condensate [22]. We note that, within this approach, the MIT shows up in the wave function in the form of a binding-unbinding transition of oppositely charged particles (empty and doubly occupied sites) [9].

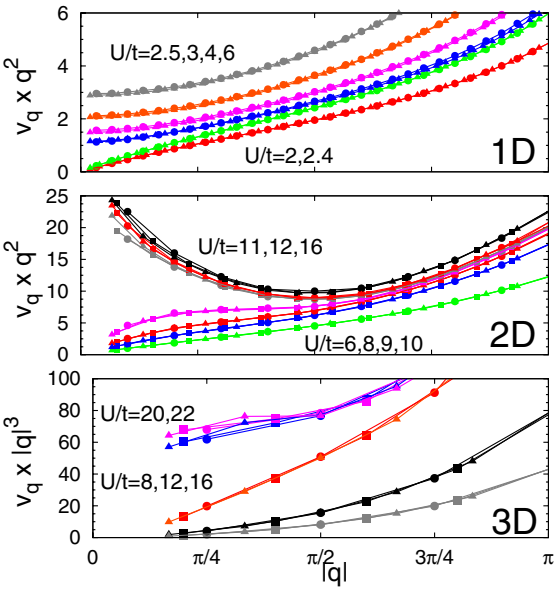

FIG. 1 (color online). Variational results for the Jastrow potential v_q multiplied by q^2 in one and two dimensions and by $|q|^3$ in three dimensions for increasing values of U/t (from bottom to top). Upper panel: 1D case for 60 (circles) and 100 (triangles) sites. Middle panel: 2D case for 20×20 (circles), 26×26 (squares), and 30×30 (triangles) clusters (along the (1, 0) direction). Lower panel: 3D case for $8 \times 8 \times 8$ (circles), $10 \times 10 \times 10$ (squares), and $12 \times 12 \times 12$ (triangles) clusters [along the (1,0,0) direction].

In order to check the validity of our approach, we compare the VMC results of the density structure factor N_q with the numerically exact ones obtained by GFMC calculations. At small q's we can generally write $N_q \sim \gamma_1|q| + \gamma_2 q^2$. In the superfluid phase, $\gamma_1 \neq 0$ while, in the Mott insulator, $\gamma_1 = 0$ and $\gamma_2 \neq 0$; see Fig. 2. In one dimension, we have evidence that γ_1 has a very sharp crossover from a finite value to zero across the MIT, suggestive of a true jump in the thermodynamic limit. Moreover, our numerical results indicate that γ_2 diverges as the MIT is approached from the insulating side (this is particularly evident from the GFMC results). Within the variational approach, this behavior follows from $v_q \sim \beta_{1\mathrm{D}}/q^2$ in the insulating phase with $\beta_{1\mathrm{D}} \to 0$ at the transition. In conclusion, the 1D MIT can be located at

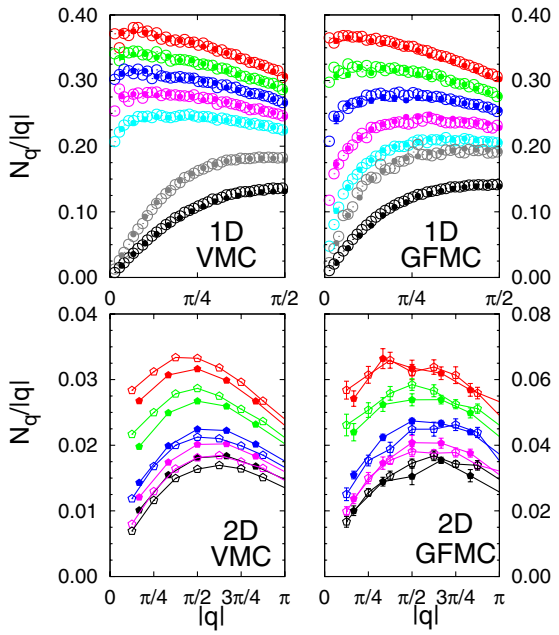

FIG. 2 (color online). Density structure factor N_q divided by $|q|$ calculated with variational Monte Carlo (left panels) and GFMC (right panels) simulations in one dimension (upper panels) and two dimensions (lower panels). In one dimension, $L = 60$ (full symbols) and $L = 150$ (empty symbols) and $U/t = 1.6, 1.8, 2, 2.2, 2.4, 2.5$. and 3. In two dimensions, $L = 12 \times 12$ (closed symbols) and 16×16 (open symbols) for the variational calculation ($U/t = 10$, 10.2, 10.4, 10.6, and 10.8) and for the GFMC calculation ($U/t = 8$, 8.2, 8.4, 8.6, and 8.8). All cases are shown from top to bottom for increasing values of U/t.

$U_c/t \simeq 2.45 \pm 0.05$ in the VMC method, whereas the GFMC method gives $U_c/t \simeq 2.1 \pm 0.1$ (in agreement with previous calculations of Refs. [23,24]), showing that the wave function (2) is not only qualitatively but also quantitatively correct.

The density structure factor N_q displays quite distinct long-wavelength behaviors for weak and strong interaction also in 2D; see Fig. 2. The VMC structure factor goes like $N_q \sim \gamma_1|q| + \gamma_2 q^2$, for $U/t \lesssim 10.3$, while above we find $N_q \sim \gamma_2 q^2$. The critical value of the on-site interaction is slightly different from the GFMC one, $U_c/t \simeq 8.5$, which agrees with Ref. [25]. In spite of slightly different values of U_c, the qualitative behavior across the MIT is similar both in VMC and in GFMC. Differently from one dimension, approaching the MIT in two dimensions, $\gamma_1 \to 0$ while $\gamma_2 \neq 0$ is smooth across the transition.

Even more interesting is the 3D case. Here, the GFMC is severely limited by small sizes; hence, we just discuss the variational results. As we mentioned, the optimal Jastrow potential turns from $v_q \sim \alpha/|q|$ in the superfluid phase, into $v_q \sim \beta_{3D}/|q|^3$ in the Mott insulator (see Fig. 1). The sudden change of behavior allows us to locate the transition around $U_c \simeq 18t$, which is close to the critical value of recent Monte Carlo simulations in three dimensions [26]. Even though $v_q \sim 1/|q|^3$, the structure factor in the Mott insulator has the correct $N_q \sim q^2$ behavior. In turn, this implies that Eq. (3) does not hold, not even for $|q| \to 0$, which is quite unexpected. In order to prove more firmly that $v_q \sim \beta_{3D}/|q|^3$ can indeed lead to $N_q \sim q^2$, we have calculated the latter with a nonoptimized wave function of the form (2) with $v_q \sim \beta_{3D}/|q|^3$ and for different values of β_{3D}. As shown in Fig. 3, for small β_{3D} we have $N_q \sim |q|^3$, implying that Eq. (3) is qualitatively correct. However, above a critical β^*_{3D}, the behavior turns into $N_q \sim q^2$, signaling a remarkable breakdown of Eq. (3). The optimal value of β_{3D} that we get variationally at the MIT is larger than β^*_{3D}, confirming our finding $N_q \sim q^2$. We note that the change of behavior as a function of β_{3D} is consistent with the binding-unbinding phase-transition recently uncovered in a classical 3D gas with $1/|q|^3$-potential [27].

Let us now come back to our original motivation concerning the dynamical properties across the superfluid-insulator transition. Although our variational wave function is meant only to describe the ground state, it can also provide important insights into the structure of the excitation spectrum. One can easily prove that the following expression holds in model (1) [13]:

$$E(q) = 2\frac{\langle -T\rangle}{DN_q}\sum_{i=1}^{D}\sin^2\left(\frac{q_i}{2}\right) = \frac{\int d\omega\, \omega S(q,\omega)}{\int d\omega S(q,\omega)}, \qquad (4)$$

where $\langle T\rangle$ is the average value of the hopping term in the Hamiltonian (1), the sum is over the spatial directions, $D = 1, 2, 3$ is the space dimensionality, and $S(q, \omega)$ the dynamical structure factor. $E(q)$ is the first moment of $S(q, \omega)$ and can be regarded as the *average energy* of density excitations, which is therefore directly accessible

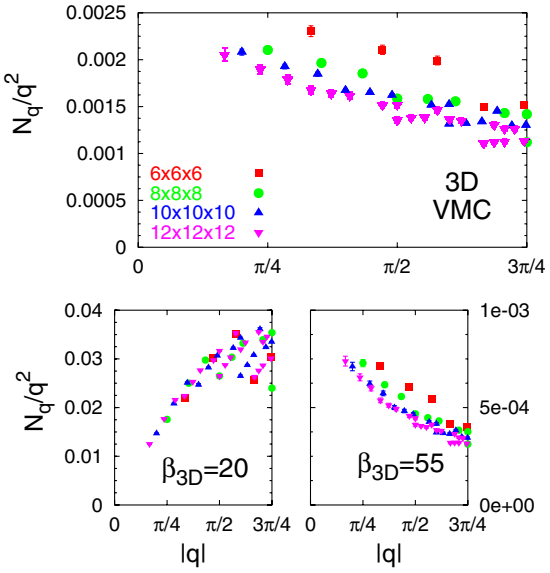

FIG. 3 (color online). Upper panel: Density structure factor N_q calculated by the variational Monte Carlo calculations for three dimensions and $U/t = 20$. Lower panels: N_q for nonoptimized wave functions with $v_q \sim \beta_{3D}/|q|^3$ for two values of β_{3D}.

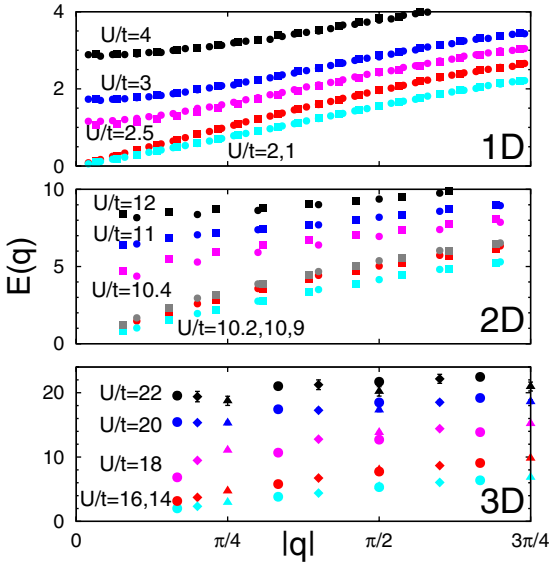

FIG. 4 (color online). Variational results for the average energy of density excitations $E(q)$ of Eq. (4) in one, two, and three dimensions.

through our variational calculation. In the superfluid phase $E(q) \propto q$ at small q, while $E(q)$ develops a finite gap, i.e., $E(0) \neq 0$, in the Mott insulator, which is an upper bound of the actual Mott-Hubbard gap. In 1D this gap seems to vanish at the MIT, in agreement with the Berezinskii-Kosterlitz-Thouless scenario; see Fig. 4. On the contrary, both in two and three dimensions, we find that $E(0)$ is finite and of order U everywhere in the Mott insulating side, even right at the MIT; see Fig. 4. This implies that high-energy excitations exist in the Mott insulator and carry most of the spectral weight. Also interesting is the behavior of the linear slope of $E(q)$ within the superfluid phase as the MIT is approached. We recall that, assuming for the structure factor the small-q expression $N_q = \gamma_1|q| + \gamma_2 q^2 + O(q^3)$, γ_1 is finite at the MIT in 1D, while it vanishes in two and three dimensions. Moreover, as the MIT is approached, γ_2 diverges in one dimension but stays finite in two and three dimensions. Since the hopping energy is finite and continuous across the transition, it follows that in two and three dimensions the linear slope of $E(q)$ should diverge at the MIT, although our numerical evidence is more clear-cut in three dimensions than in two. Excluding the possibility that the sound velocity diverges at the MIT, we must conclude that the spectral weight is gradually transferred from the sound mode to high-energy excitations that exist already in the superfluid phase and are smooth across the MIT, suggestive of preformed Mott-Hubbard bands. These results are actually consistent with the broad continuum of high-energy excitations beyond the sound mode observed experimentally in the superfluid phase [3].

In conclusion we have shown that a long-range Jastrow potential does allow for a faithful variational description of a Mott transition in the bosonic Hubbard model. The average energy of the density excitations, that is accessible by our calculation, suggests in two and three dimensions that preformed Hubbard bands coexist with sound modes in the superfluid phase near the Mott transition and carry most of the spectral weight in the insulator. This is an interesting and also surprising result, that bears a lot of similarities with the MIT in electronic systems [4], but is not accounted for by most accepted theories of the superfluid to Mott-insulator transition in bosonic systems. In analogy with the bosonic example, we expect that a singular Jastrow potential $v_q \sim 1/|q|^3$ is necessary to describe the 3D Mott transition in fermionic models.

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