Superfluid to Mott-insulator transition in Bose-Hubbard models

Manuela Capello,1 Federico Becca,2,3 Michele Fabrizio,2,3,4 Sandro Sorella,2,3
1 Laboratoire de Physique Théorique, Université Paul Sabatier, CNRS, 31400 Toulouse, France
2 International School for Advanced Studies (SISSA), I-34014 Trieste, Italy
3 CNR-INFM-Democritos National Simulation Centre, Trieste, Italy
4 International Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy
(Dated: February 1, 2008)

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 evidences that, across the transition, most of the spectral weight is concentrated at high energies, suggestive of pre-formed Mott-Hubbard side-bands. This result is compatible with the experimental data by Stoferle et al. [Phys. Rev. Lett. 92, 130403 (2004)].

PACS numbers: 71.10.Hf, 71.27.+a, 71.30.+h

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 $U$ develops already on the superfluid side of the MIT, akin to what is predicted to occur in electronic systems. [1] Although these evidences are not incompatible with the accepted theory of the critical behavior across the superfluid-to-insulator transition, [3] they clearly demand for a more detailed comprehension that must include also 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. [5, 12, 13, 14] 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 intend to 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, 9, 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 in optical lattices can be modeled by the Hubbard Hamiltonian: [5, 12, 13, 14]

$$\mathcal{H} = -\sum_{ij,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + H.c. + U/2 \sum_i n_i (n_i - 1), \quad (1)$$

where $a_{i\sigma}^\dagger$ ($a_{i\sigma}$) creates (annihilates) a particle at site $i$ with integer spin $\sigma = -S, \ldots, S$, and $n_i = \sum_{\sigma} a_{i\sigma}^\dagger a_{i\sigma}$. The Hubbard model (1) at integer filling has generally two different phases: one superfluid, for $U < U_c$, and the other insulating above $U_c$. In this work, we shall focus on the spinless case and attempt 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 turns out to be 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. [13, 16]

Recently, an extension of the Gutzwiller wave function has been proposed [8, 10] that proved to be very accurate to describe an electronic MIT in 1D. [8, 10] Here we apply the same variational approach to the $S = 0$ 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

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

where $|\Phi_0\rangle$ is the non-interacting fully-condensed wave function

$$\Phi_0 = \prod_{i} \left( \sum_{\sigma} \frac{1}{2} \left(1 + \sigma \right) a_{i\sigma} \right). \quad (3)$$
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, $v_{i,j} = \nu(|R_i - R_j|)$, are independently optimized by a Variational Monte Carlo (VMC) minimization of the total energy.\cite{17} In the following, we will denote by $\rho_\nu$ and $v_\nu$ the Fourier transforms of the boson-density $\nu_i$ 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 $\delta$ is the vector that connects nearest-neighbor sites.\cite{18} This term is kept just to improve the variational accuracy (mainly in 2D and 3D) but does not introduce important correlation effects, that are instead contained only in the long-range tail of the two-body Jastrow potential $v_{i,j}$. Both the Jastrow factor and the many-body operator $\xi$ commute with the particle number, hence belongs to the Fock space with $N = L$ bosons.

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 $\nu$, which is the novel ingredient with respect to the conventional Gutzwiller wave function. In the superfluid phase, a long-range Jastrow potential is surely needed to restore the correct small-$q$ behavior of the static density structure factor, 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

$$N_q = \frac{\langle \Phi_0 | \rho_{-q} \rho_q | \Phi_0 \rangle}{1 + \gamma v_\nu N_q^0} \tag{3}$$

holds with $\gamma = 2$.\cite{19} and because the non-interacting $N_q^0 = \langle \Phi_0 | \rho_{-q} \rho_q | \Phi_0 \rangle \sim \text{const}$, it follows that $v_\nu \sim 1/|q|$. Assuming that the expression $\langle \rangle$ remains valid for $|q| \rightarrow 0$ even in the Mott insulating phase, one might be tempted to believe that $v_\nu \sim 1/q^2$ 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 $\nu$ could not describe any bosonic insulator in 3D, since $v_\nu \sim 1/q^2$ is not sufficient to empty the condensate fraction.\cite{20} Indeed, as shown below, the optimized variational wave function $\nu$ has a more diverging $v_\nu \sim 1/|q|^3$ in the 3D Mott insulator, although $N_q \sim q^2$, implying that the formula $\langle \rangle$ does not generally hold.

In Fig. 1 we draw the optimized Jastrow potential $\nu$.

For any dimension, the MIT is clearly signaled by the sudden change in the small-$q$ behavior of $v_\nu$. On the one hand, the superfluid phase is always described by $v_\nu \sim \alpha/|q|$, with $\alpha$ increasing with $U$. On the other hand, the Mott insulator has a much more diverging $v_\nu$. In 1D we recover the $v_\nu \sim 1/q^2$ behavior, like in the fermionic case.\cite{8} In 2D, the leading behavior of the Jastrow po-
that the wave function (2) is not only qualitatively but also quantitatively consistent with previous calculations of Ref. [22, 23], showing that the superfluid phase, into the MIT is similar both in VMC and in GFMC. Differently from 1D, approaching the MIT in 2D, $\gamma_1 \to 0$ 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 and, therefore, 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 to locate the transition around $U_c/t \approx 18$, which is close to the critical value of recent Monte Carlo simulations in 3D. [25] Even though $v_q \sim 1/|q|^3$, the structure factor in the Mott insulator has the correct behavior $|q| \sim q^2$. In turns 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 non-optimized wave function of the form (2) with $v_q \sim \beta_{3D}/|q|^3$ and for different values of $\beta_{3D}$. As shown in Fig. 3 for small $\beta_{3D}$ we have $N_q \sim |q|^3$, implying that Eq. (3) is qualitatively correct. However, above a critical $\beta_{3D}^{\text{crit}}$, the behavior turns into $N_q \sim q^2$, signaling a remarkable breakdown of Eq. (3). The optimal value of $\beta_{3D}$ that we get variationally at the MIT is larger than $\beta_{3D}^{\text{crit}}$, confirming our variational finding $N_q \sim q^2$. We note that the change of behavior as a function of $\beta_{3D}$ is consistent with the numerically exact ones obtained by GFMC. At $U_c/t=20$, whereas GFMC gives $U_c/t\approx 2.1 \pm 0.1$ (in agreement with previous calculations of Ref. [22, 23]), 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. 4. 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, $U_c/t \approx 8.5$, which agrees with Ref. [24]. 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 1D, approaching the MIT in 2D, $\gamma_1 \to 0$ 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 and, therefore, 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 to locate the transition around $U_c/t \approx 18$, which is close to the critical value of recent Monte Carlo simulations in 3D. [25] Even though $v_q \sim 1/|q|^3$, the structure factor in the Mott insulator has the correct behavior $N_q \sim q^2$. In turns 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 non-optimized wave function of the form (2) with $v_q \sim \beta_{3D}/|q|^3$ and for different values of $\beta_{3D}$. As shown in Fig. 3 for small $\beta_{3D}$ we have $N_q \sim |q|^3$, implying that Eq. (3) is qualitatively correct. However, above a critical $\beta_{3D}^{\text{crit}}$, the behavior turns into $N_q \sim q^2$, signaling a remarkable breakdown of Eq. (3). The optimal value of $\beta_{3D}$ that we get variationally at the MIT is larger than $\beta_{3D}^{\text{crit}}$, confirming our variational finding $N_q \sim q^2$. We note that the change of behavior as a function of $\beta_{3D}$ is consistent with the numerically exact ones obtained by GFMC. At $U_c/t=20$, whereas GFMC gives $U_c/t\approx 2.1 \pm 0.1$ (in agreement with previous calculations of Ref. [22, 23]), 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. 4. 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, $U_c/t \approx 8.5$, which agrees with Ref. [24]. 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 1D, approaching the MIT in 2D, $\gamma_1 \to 0$ 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 and, therefore, 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 to locate the transition around $U_c/t \approx 18$, which is close to the critical value of recent Monte Carlo simulations in 3D. [25] Even though $v_q \sim 1/|q|^3$, the structure factor in the Mott insulator has the correct behavior $N_q \sim q^2$. In turns 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 non-optimized wave function of the form (2) with $v_q \sim \beta_{3D}/|q|^3$ and for different values of $\beta_{3D}$. As shown in Fig. 3 for small $\beta_{3D}$ we have $N_q \sim |q|^3$, implying that Eq. (3) is qualitatively correct. However, above a critical $\beta_{3D}^{\text{crit}}$, the behavior turns into $N_q \sim q^2$, signaling a remarkable breakdown of Eq. (3). The optimal value of $\beta_{3D}$ that we get variationally at the MIT is larger than $\beta_{3D}^{\text{crit}}$, confirming our variational finding $N_q \sim q^2$. We note that the change of behavior as a function of $\beta_{3D}$ is consistent with the numerically exact ones obtained by GFMC. At $U_c/t=20$, whereas GFMC gives $U_c/t\approx 2.1 \pm 0.1$ (in agreement with previous calculations of Ref. [22, 23]), 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. 4. 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, $U_c/t \approx 8.5$, which agrees with Ref. [24]. 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 1D, approaching the MIT in 2D, $\gamma_1 \to 0$ while $\gamma_2 \neq 0$ is smooth across the transition.
tent with the binding-unbinding phase transition recently uncovered in a classical 3D gas with $1/|\mathbf{q}|^3$-potential. 26

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):

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

where $\langle T \rangle$ is the average value of the hopping, 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 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 Berezinski-Kosterlitz-Thouless scenario, see Fig. 4. On the contrary, both in 2D and 3D, 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 $N_q = \gamma_1 |q| + \gamma_2 q^2 + O(q^3)$, $\gamma_1$ is finite at the MIT in 1D, while it vanishes in 2D and 3D. Moreover, as the MIT is approached, $\gamma_2$ diverges in 1D but stays finite in 2D and 3D. Since the hopping energy is finite and continuous across the transition, it follows that in 2D and 3D the linear slope of $E(q)$ should diverge at the MIT, although our numerical evidence is more clearcut in 3D than in 2D. 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 pre-formed Mott-Hubbard side bands. These results are actually consistent with the experimental data of Ref. 3.

In conclusion we have demonstrated 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 charge-density excitations, that is accessible by our calculation, suggests in two and three dimensions that pre-formed Hubbard side-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, too, all the more reason when realistic Coulomb interaction is taken into account, in which case a Jastrow potential $1/|q|^2$ is necessary already in the metal to reproduce the proper long-wavelength behavior.

We acknowledge useful discussions with D. Poilblanc and T. Senthil. This work has been partially supported by CNR-INFM and COFIN 2004 and 2005.

[1] N.F. Mott, Metal Insulator Transition (Taylor and Francis, London, 1990).
[2] M. Greiner et al., Nature (London) 415, 39 (2002).
[3] T. Stoferle et al., Phys. Rev. Lett. 92, 130403 (2004).
[4] A. Georges et al., Rev. Mod. Phys. 68, 13 (1996).
[5] M.P.A. Fisher et al., Phys. Rev. B 40, 546 (1989).
[6] S.R. Huber et al., Phys. Rev. B 75, 085106 (2007).
[7] S.R. Clark and D. Jakšch, Phys. Rev. A 70, 063612 (2004).
[8] M. Capello et al., Phys. Rev. Lett. 94, 026406 (2005).
[9] M. Capello et al., Phys. Rev. B 73, 245116 (2006).
[10] M. Capello et al., Phys. Rev. B 72, 085121 (2005).
[11] M. Calandra Buonaura and S. Sorella, Phys. Rev. B 57, 11446 (1998).
[12] D. Jakšch et al., Phys. Rev. Lett. 81, 3108 (1998).
[13] R. Roth and K. Burnett, J. Phys. B 37, 3893 (2004).
[14] B. Damski and J. Zakrzewski, Phys. Rev. A 74, 063609 (2006).
[15] D.S. Rokhsar and B.G. Kotliar, Phys. Rev. B 44, 10328 (1991).
[16] W. Krauth, M. Caffarel, and J.P. Bouchaud, Phys. Rev. B 45, 3137 (1992).
[17] S. Sorella, Phys. Rev. B 71, 241103 (2005).
[18] T.A. Kaplan, P. Horsch, and P. Fulde, Phys. Rev. Lett. 49, 889 (1982).
[19] T. Gaskell, Proc. Phys. Soc. 77, 1182 (1961); L. Reatto and G.V. Chester, Phys. Rev. 155, 88 (1967).
[20] L. Reatto, Phys. Rev. 183, 334 (1969).
[21] In 1D, even $v_q \sim 1/|q|^3$ is sufficient to completely suppress the condensate fraction, as expected from Ref. 20.
[22] G.G. Batrouni, R.T. Scalettar, and G.T. Zimanyi, Phys. Rev. Lett. 65, 1765 (1990).
[23] T.D. Kühner and H. Monien, Phys. Rev. B 58, R14741 (1998).
[24] W. Krauth and N. Monien, Phys. Rev. B 58, 14741 (1998).
[25] B. Capogrosso-Sansone, N.V. Prokof’ev, and B.V. Svistunov, Phys. Rev. B 75, 134302 (2007).
[26] S. Kragset, A. Sudbo, and F.S. Nogueira, Phys. Rev. Lett. 92, 186403 (2004).