First Mott lobe of bosons with local two- and three-body interactions

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Using the density matrix renormalization group method, we determine the phase diagram of the Bose-Hubbard model with local two- and three-body interactions, describing polar molecules in one-dimensional optical lattices. The difference in the block von Neumann entropy with different system sizes was used to establish the critical points. We found that the quantum critical point position increases with the three-body interaction. We show that the model studied is in the same universality class as the model with pure two-body interactions.

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I. INTRODUCTION

The intense investigation of cold atoms loaded into an optical lattice has made possible the experimental observation of quantum phase transitions in degenerate gases. For instance, Greiner *et al.* [1] observed a quantum phase transition from a superfluid to a Mott insulator phase by loading ^{87}Rb atoms into a three-dimensional (3D) optical lattice potential. Working with the same atoms, Stöferle *et al.* [2] used an optical lattice to realize a strongly interacting Bose gas in one spatial dimension (1D), and they study the transition between the Mott insulator and superfluid phases in the crossover regime from 1D to 3D.

The above experimental results were reasonably described using the Bose-Hubbard model in any dimension. In one dimension, this model with pure two-body interactions has been intensively studied [3–7]. A compressible superfluid state or a Mott insulator state can be obtained, and we know that the model is in the universality class of the XY spin model so that there is a Kosterlitz-Thouless phase transition with the Tomonaga-Luttinger parameter $K = 1/2$, and the gap is exponentially small in the vicinity of the critical point. Recently, more precise calculation found that the critical point is located at $t_c = 0.305 \pm 0.001$ [7].

The most common interaction effects in condensed matter physics are due to two-body interactions, and the other higher-order many-body interactions are negligible corrections, usually treated within perturbation theory. However, Büchler *et al.* [8] showed that polar molecules in optical lattices can be tuned to a regime where the three-body interactions are dominant, opening a route for theoretical and experimental research of new exotic quantum phases [9,10].

In this Brief Report, we study 1D bosons interacting by local two- and three-body terms motivated by the recent mean-field calculations of Chen *et al.* [11] and Zhou *et al.* [12], who found that the Mott-insulating surfaces rotate with respect to a fixed point.

II. MODEL

Using the single-band approximation [13], bosons confined in optical lattices can be described by the Hamiltonian

$$H = -t\sum_i (b_i^\dagger b_{i+1} + \text{H.c.}) + \frac{U}{2}\sum_i n_i(n_i-1) + \frac{W}{6}\sum_i n_i(n_i-1)(n_i-2), \qquad (1)$$

where, in standard notation, i varies along the sites of a one-dimensional lattice of size L, $b_i^\dagger(b_i)$ creates (annihilates) a boson at site i, and $n_i = b_i^\dagger b_i$ is the number of particles on site i. The first term in the Hamiltonian (1) is the kinetic energy with strength t (hopping amplitude), the second term considers the on-site two-body repulsion (U), and the last term stems from the short-range interaction between three bosons, while the parameter W characterizes its strength. The energy scale is set by choosing $U = 1$, and we assume that the lattice constant is equal to 1.

Without three-body interactions, it is well known that at integer filling the Bose-Hubbard model shows a quantum phase transition at a critical value of $t_c = (t/U)_c$ from a superfluid phase ($t/U > t_c$), in which the atoms are delocalized, to a Mott insulating phase ($t/U < t_c$) in which the atoms are localized. The latter phase has a finite gap for single-particle excitations, which is given by $\Delta\mu(L) = E_0(L,N+1) + E_0(L,N-1) - 2E_0(L,N)$, where $E_0(L,N)$ is the ground-state energy for L sites and N particles. At the thermodynamic limit, $N,L \to \infty$ and $\rho = N/L$ integer, a finite gap is expected, i.e., $\Delta\mu = \lim_{N,L\to\infty} \Delta\mu(L) > 0$.

The superfluid phase is gapless and the low-energy physics of the 1D Bose-Hubbard model can be described as a Luttinger liquid, which is a conformal field theory with central charge $c = 1$. Using conformal field theory, it was possible to find an expression for the von Neumann entropy with different boundary conditions [14].

Now we define the von Neumann entropy. For this, we consider a system with L sites divided into two parts: A with l sites ($l = 1,\dots,L$) and B with $L - l$ sites. If the system is in a pure state, the von Neumann entropy of the block A is defined by $S_L(l) = \text{Tr}\rho_A \ln \rho_A$, where $\rho_A = \text{Tr}_B\rho$ and ρ is the density matrix of the whole system.

The behavior of the von Neumann entropy (block entropy) $S_L(l)$ as a function of l depends on whether the ground state is critical or not, i.e., the von Neumann entropy saturates (diverges) if the system is gapped (gapless), namely [14,15],

$$S_L(l) = \begin{cases} \frac{c}{3\eta}\ln\left[\frac{\eta L}{\pi}\sin\left(\frac{\pi l}{L}\right)\right] + \theta, & \text{critical,} \\ \frac{c}{3\eta}\ln[\zeta_L] + \theta', & \text{noncritical,} \end{cases} \qquad (2)$$

where c is the central charge, ζ_L is the correlation length, and $\eta = 1$ ($\eta = 2$) for periodic (open) boundary conditions. The constants θ and θ' are nonuniversal and model dependent.

Läuchli and Kollath [16] proposed the estimator $\Delta S_{\rm LK}(L) = S_L(L/2) - S_{L/2}(L/4)$ to determine the critical point (t_c) of the Bose-Hubbard model with two-body interactions, which separates the Mott insulating phase and the superfluid phase. According to (2) as $L \to \infty$, we should have

$$\Delta S_{LK}(L) = \begin{cases} \frac{c}{3\eta}\ln(2), & t \geqslant t_c \\ 0, & t < t_c. \end{cases} \quad (3)$$

They found that an appropriate scaling plot of the estimator $\Delta S_{\rm LK}(L)$ provides good results with respect to the location of the critical point in the model.

In order to determine the ground-state energy and the von Neumann entropy of the Bose-Hubbard model with two- and three-body interactions, we used the density matrix renormalization group (DMRG) method with open boundary conditions ($\eta = 2$) [17]. We used the finite-size algorithm for sizes up to $L = 512$; we considered a truncated Hilbert space with five states by site and fixed the density $\rho = N/L = 1$. We kept up to $m = 600$ states per block and obtained a discarded weight around 10^{10} or less.

III. RESULTS

In Fig. 1, we show the phase diagram for the first Mott lobe ($\rho = 1$) of the model, for three different values of the three-body interaction parameter ($W/U = 0.0$, 3.0, and 7.0). The symbols are the particle (hole) excitation energy at the thermodynamic limit extrapolated from $\mu^p(L) = E_0(L,N+1) - E_0(L,N)$ [$\mu^h(L) = E_0(L,N) - E_0(L,N-1)$] for $L \leqslant 128$. When $W/U = 0.0$, we observe a Mott insulator phase surrounded by a superfluid phase and we reproduce the well-known phase boundaries of the Bose-Hubbard model with only two-body interactions, which were determined using different analytical and numerical methods [3–7]. For finite values of W/U, we also observe a superfluid phase surrounding an incompressible Mott insulator phase; however, the three-body interactions increase the insulating area in the phase diagram and move the tip of the Mott insulator for bigger values. This result is expected because the additional local three-body interactions help to localize the particles, and we need higher energy to delocalize it. These findings don't appear in the previous mean-field treatments of this problem [11,12] and motivated the present study. They showed that for $\rho = 1$ the Mott insulator area is independent of the three-body interactions; therefore the critical point will be that of the model with pure two-body interactions for all values of W/U. We observe that only in the strong coupling regime ($t \to 0$) are the critical points independent of the three-body interaction.

We see in Fig. 1 that the tip of the Mott insulator phase moves as the three-body interaction increases; now we want to determine the quantum critical point for each value of W/U. For pure two-body interactions ($W/U = 0$), this task was done based on *a priori* knowledge that the quantum phase transition is the Kosterlitz-Thouless type [5–7]. However, in recent years it has been shown that it is possible to determine quantum critical points calculating the ground-state entanglement [16,18,19], and we chose this method to determine the quantum critical points of the Bose-Hubbard model with two- and three-body interactions. Namely, we calculate the block entropy $S_L(l)$ and the estimator $\Delta S_{\rm LK}(L)$ for several combinations of the parameters.

The behavior of the block entropy $S_L(l)$ as a function of the block size l is shown in Fig. 2. In this figure we fixed $W/U = 7.0$ and considered three different values of the hopping ($t/U = 0.25$, 0.30, and 0.5). At the strong coupling limit $t \to 0$ the entanglement vanishes because the ground state is separable; i.e., this is given by a product of local states with one particle. For $t/U = 0.25$ the block entropy is not zero and we see that this increases and saturates quickly, showing that the ground state has a finite correlation length, i.e., the system is in a Mott insulator phase (see Fig. 1). When the hopping increases, the description of the ground state in terms of a product of local states is harder, and the entanglement increases, as can be seen for $t/U = 0.30$ and 0.50. We observe that the block entropy diverges with l for $t/U = 0.50$; this fact indicates that the system is in a critical

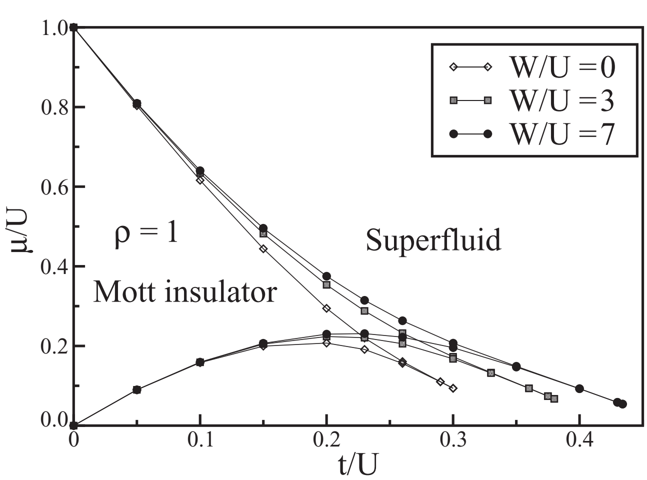

FIG. 1. Phase diagram of the Bose-Hubbard model with two- and three-body interactions. We show the phase boundaries for three different values of $W/U = 0.0, 3.0$, and 7.0.

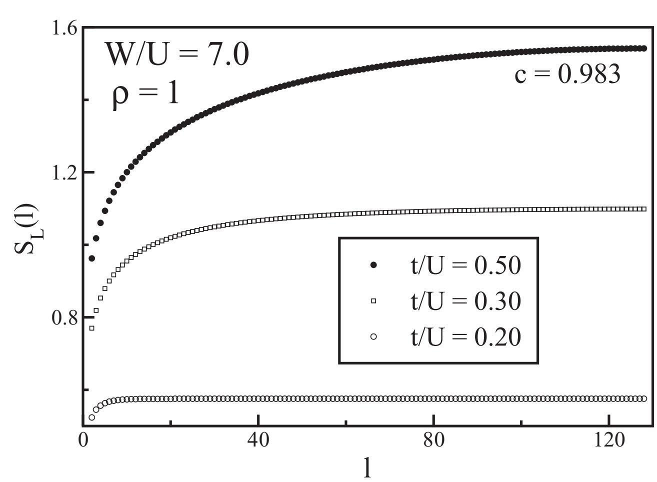

FIG. 2. The block entropy $S_L(l)$ as a function of l for a system with size $L = 256$ and $W/U = 7.0$. The hopping parameters are $t/U = 0.25, 0.30$, and 0.5.

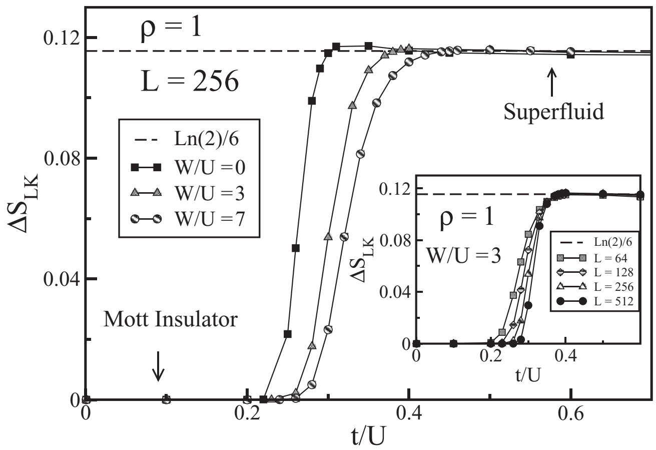

FIG. 3. Estimator ΔS_{LK} as a function t/U for different values of three-body interaction $W/U = 0,3$, and 7. Here we fixed $L = 256$. Inset: Estimator ΔS_{LK} vs t/U for three-body interaction $W/U = 3$, and different system lengths $L = 64,128,256$, and 512.

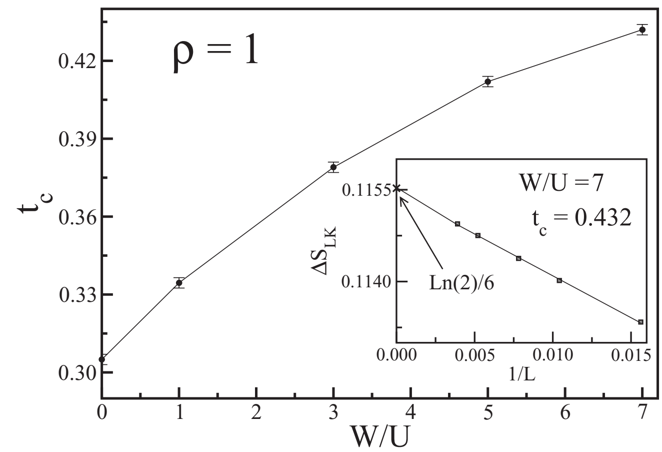

FIG. 4. Quantum critical point position as a function of W/U for the Bose-Hubbard model with two- and three-body interactions. Inset: Estimator ΔS_{LK} as a function of $1/L$ for $W/U = 7$ and $t/U = 0.432$.

region. We fit the DMRG data to the conformal field theory expression for the block entropy (2), and we find that the central charge is $c = 0.983$ for $t/U = 0.50$. We observe that this value of the central charge is closer to 1, the value for pure two-body interactions [16]. The curve for $t/U = 0.30$ shows an intermediate case inside the Mott insulator phase in which the block entropy increases but saturates at the end.

For a fixed three-body interaction $W/U = 3$, the estimator $\Delta S_{\mathrm{LK}}(L)$ as a function of t/U is shown in the inset of Fig. 3. We consider different system sizes L from 32 up to 512 sites, and we observe that in the strong coupling ($t \to 0$) the estimator vanishes. When the hopping increases, the estimator remains constant and equal to $\Delta S_{\mathrm{LK}}(L) = 0$ until it reaches a certain hopping value; then the estimator grows rapidly in a small region up to the limiting value ln(2)/6, remaining near to it. When the system size increases, the hopping for which $\Delta S_{\mathrm{LK}}(L) \neq 0$ moves to the right and the growth region decreases; thus the curve tends to a step function as a function of t/U according to (3). When the estimator is zero, the ground state has a finite correlation length; i.e., we have a Mott insulator phase at the left side, whereas at the right side the estimator remains around the value ln(2)/6, which indicates that the ground state is superfluid. The deviation from the value ln(2)/6 observed in Fig. 3 is the open boundaries effect, and is not captured in the conformal field theory [16].

In Fig. 3, we observe that the behavior of the estimator as a function of t/U for other values of the three-body interaction is the same as mentioned above. We see that the curve moves to the right as the three-body interaction increases in accordance with that observed in Fig. 1. As mentioned by Läuchli and Kollath [16], the critical point will be the first value for which the estimator reaches (at the thermodynamic limit) the value ln(2)/6 when the hopping increases from zero. For instance, we clearly observe that the critical point for $W/U = 0$ will be around $t_c(W = 0) \approx 3.0$ in accordance with previous estimations [6,7]. From Fig. 3, we note that the position of the quantum critical points will increase with W/U.

The estimator ΔS_{LK} as a function of $1/L$ for the three-body interaction $W/U = 7$ and hopping parameter $t/U = 0.432$ is shown in the inset of Fig. 4. When the system size increases, we can see that the estimator grows and we consider that the lattice size dependence is $\Delta S_{\mathrm{LK}}(L) = a + b/L + c/L^2$. For this hopping value, we found that the estimator reaches the value ln(2)/6 at the thermodynamic limit, for the first time starting at zero; therefore, this hopping value corresponds to the transition point, i.e., the quantum critical point for $W/U = 7$ is $t_c = 0.432 \pm 0.001$. Following the procedure described above, we found the critical points for other values of the three-body interaction. In Fig. 4, we show the position of the quantum critical points as a function of the three-body interactions W/U. We observe that the quantum critical points increases with W/U, in accordance with Fig. 1. We believe that this is due to the quantum fluctuations, which increase the effect of the three-body interaction term. The above result contradicts the findings of Chen *et al.* [11] and Zhou *et al.* [12], who found that for density $\rho = 1$ the critical points are independent of the three-body interaction.

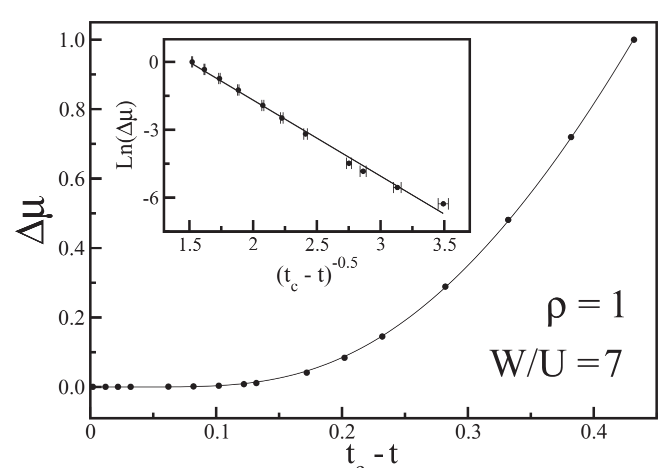

FIG. 5. Energy gap as a function of $t_c - t$ for $\rho = 1$ and $W/U = 7$. Inset: ln $\Delta\mu$ vs $1/\sqrt{t_c - t}$. Here, the points are DMRG results, and adjustments to the Kosterlitz-Thouless transition are shown by lines.

Now, we know that the Bose-Hubbard model with two- and three-body interactions presents two phases: a superfluid one and a Mott insulator one. But how does the quantum phase transition happen? To answer this question we can use the critical point t_c calculated with the estimator and try to fit the gap to a special function [20]. One possibility is the function that describes the well-known Kosterlitz-Thouless transition, for which the gap follows $\Delta\mu = A \exp[-b/\sqrt{t_c - t}]$, where A and b are constants.

In Fig. 5 we display the energy gap as a function of $t_c - t$ when $W/U = 7$. We observe that the gap grows slowly in a spread region, then increases quickly, and finally the tendency is almost linear. The line is the fit to the gap expression, showing a good match between the DMRG points and the line. In the inset of Fig. 5, we plot $\ln \Delta\mu$ as a function of $1/\sqrt{t_c - t}$; we observe a linear tendency, which indicates that the Kosterlitz-Thouless behavior is suitable for describing the closing of the gap. The above results and the central charge ($c = 1$) show us that the Bose-Hubbard model with two- and three-body interactions is in the same universality class as the model with pure two-body interactions.

IV. CONCLUSIONS

We used the density matrix renormalization group method to study the Bose-Hubbard model with two- and three-body interactions. This model presents a Mott insulator and a superfluid phase, and we determined the phase diagram for different values of the three-body interactions, which increases the Mott insulator area in the phase diagram. To find the critical points, we calculated the block von Neumann entropy and used the previously defined estimator $\Delta S_{\rm LK}$, which tends to a step function at the critical point. We found that the position of the critical points increases as a function of the three-body interaction, in contradiction to the previous mean-field results. With the obtained critical points, we show that the gap of the model closes following the Kosterlitz-Thouless tendency in the same way as the model with pure two-body interactions.

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