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Phys. Rev. A **87**, 043606 — Published 8 April 2013

DOI: [10.1103/PhysRevA.87.043606](https://doi.org/10.1103/PhysRevA.87.043606)

# Scaling of the gap, fidelity susceptibility, and Bloch oscillations across the superfluid to Mott insulator transition in the one-dimensional Bose-Hubbard model

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(Dated: March 26, 2013)

We investigate the interaction induced superfluid to Mott insulator transition in the one-dimensional (1D) Bose-Hubbard model (BHM) for fillings  $n = 1$ ,  $n = 2$ , and  $n = 3$  by studying the single-particle gap, the fidelity susceptibility, and the amplitude of Bloch oscillations via density matrix renormalization group (DMRG) methods. We apply a generic scaling procedure for the gap, which allows us to determine the critical points with very high accuracy. We also study how the fidelity susceptibility behaves across the phase transition. Furthermore, we show that in the BHM, and in a system of spinless fermions, the amplitude of Bloch oscillations after a tilt of the lattice vanishes at the critical points. This indicates that Bloch oscillations can serve as a tool to detect the transition point in ongoing experiments with ultracold gases.

PACS numbers: 03.75.Hh, 05.30.Rt, 64.70.qj, 03.75.Lm, 75.40.Mg

## I. INTRODUCTION

Ultracold atomic and molecular gases in optical lattices provide a unique playground for investigating quantum many-body phenomena [1, 2]. Since the seminal experiment by Greiner *et al.* [3], it has become common in such experiments to study quantum phase transitions in the presence of strong correlations. In particular, optical lattice realizations of the BHM

$$H = -J \sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{H.c.}) + \frac{U}{2} \sum_j n_j (n_j - 1), \quad (1)$$

have been shown to undergo a transition from a superfluid to a Mott-insulator as the ratio of  $U/J$  is increased in different dimensions [3–5]. In what follows, we set  $J = 1$  and  $\hbar = 1$ , so that  $U$  is measured in units of  $J$  and time  $t$  is measured in units of  $\hbar/J$ . We also set the lattice spacing  $a = 1$ , thus length is measured in units of  $a$ .

The 1D BHM, the focus of this study, is of particular interest because of the dominant role played by quantum fluctuations. From the theoretical side, it is challenging to accurately determine the critical value  $U_c$  at which the system at constant density undergoes a superfluid–Mott-insulator transition, something that, due to the lack of exact solutions for this model, is typically done utilizing computational approaches [2]. Here, the Berezinskii-Kosterlitz-Thouless (BKT) universality class of the transition makes calculations in finite systems susceptible to large finite-size effects. Insights from Luttinger liquid theory, combined with DMRG [6–9] calculations of correlation functions and extrapolations to the thermodynamic limit, have provided some of the most accurate

values of  $U_c$  to date [10, 11] (see Ref. [2] for a review). Due to the large numerical effort needed, alternative and more accurate scaling approaches to calculate  $U_c$ , which do not rely on computing correlation functions, are highly desirable. From the experimental point of view, many of the quantities used in theoretical studies to determine  $U_c$  are either difficult (e.g, the gap [4, 12–14]) or not possible to measure accurately. The task is complicated even further by inhomogeneities induced by the unavoidable confining potentials present [15–17]. Therefore, it is also highly desirable to find approaches to determine  $U_c$  that could be more easily implemented in experiments.

In this work, we address the two issues mentioned above, namely, how to accurately determine  $U_c$  within computational approaches and in experimental studies. First, we apply a recently proposed scaling approach for the gap [18] to obtain the critical point in the BHM with high accuracy and at fillings  $n = 1, 2, 3$ . Second, we investigate the behavior of the fidelity susceptibility across these transitions. The fidelity susceptibility, a quantity motivated from the field of quantum information, has recently attracted much attention as a means of identifying the presence of quantum phase transitions even if the nature of the involved phases is not known [19–30]. Finally, we discuss how to determine  $U_c$  by studying the center of mass motion during Bloch oscillations, which occur after tilting the lattice [31, 32]. This is something that can be easily implemented in ultracold gases experiments.

All equilibrium calculations are done utilizing DMRG and, out-of-equilibrium, the Krylov-variant of the adaptive time-dependent DMRG (t-DMRG) [8]. For ground state calculations, we perform 10 sweeps and keep up to  $m = 1000$  density matrix eigenstates. In order to ensure the high accuracy needed for the considerations below, we

truncate the local Hilbert space at  $n + 5$  bosons (where  $n = 1, 2$  or  $3$ ). The ground state energies obtained are converged in most cases with an absolute accuracy of  $10^{-7}$  or better. The computation of the fidelity susceptibility is, however, more demanding, and we are restricted to smaller systems. In order to reach the necessary accuracy in the overlap of the two wave functions involved, we use  $m \leq 4000$ . To study the out-of-equilibrium dynamics under a tilt, we truncate the local Hilbert space at  $n + 4$  bosons and keep up to  $m = 2500$  states in the course of the time evolution while using a time step of  $\Delta t = 0.01$ .

## II. SCALING ANALYSIS OF THE GAP

The phase transition from a Mott-insulator to a superfluid in the 1D BHM at commensurate fillings is known to be of BKT type [33]. Hence, it is accompanied by the exponential closing of the single-particle gap  $E_g \sim \exp(-b/\sqrt{U - U_c})$  ( $b$  is a parameter which is independent of  $U$ ). As a consequence of its exponential behavior, a direct study of the transition by computing the single-particle gap for finite systems is plagued by finite-size effects. This problem can be overcome by a scaling analysis of the gap, for which we follow the approach in Ref. [18], briefly described below.

The method is based on the following ansatz for the scaling of the gap in the vicinity of the phase transition,

$$LE_g(L) \times \left(1 + \frac{1}{2 \ln L + C}\right) = F\left(\frac{\xi}{L}\right), \quad (2)$$

where  $F$  is a scaling function,  $C$  is an unknown constant to be determined, and  $L$  is the system size. We emphasize two aspects of this scaling ansatz: First, it contains the logarithmic corrections that are typical for  $E_g(L)$  at the BKT transition [34, 35]. Second, it resembles the relation for the resistance (which also vanishes exponentially) in the charge-unbinding transition of the two-dimensional classical Coulomb gas, which is also of BKT type [36]. At the critical point, and in its vicinity within the superfluid region, one expects the values of  $F(\xi/L)$  to be system-size independent because of the divergence of the correlation length. Hence, the data for the rescaled gap  $E_g^*(L) = LE_g(L) [1 + 1/(2 \ln L + C)]$  for different system sizes  $L$  will be independent of  $L$  in this region. Furthermore, the curves  $E_g^*(L)$  vs  $\xi/L$  for several values of  $L$  and  $U$  should collapse onto a unique curve representing  $F$ . Equivalently, one can reformulate the relation in Eq. (2) by taking the logarithm of the argument of  $F$  and considering a different function  $f$  with argument  $x_L = \ln L - \ln \xi$ .

We determine the critical point by adjusting the parameters  $U_c$ ,  $b$ , and  $C$ . In the procedure, we look for the best collapse of the curves  $E_g^*(L)$  vs  $x_L$  for different values of  $U$  and  $L$ . This is done by representing the function  $f$  with a selected high-degree polynomial (eighth degree in our case) such that the results are independent of the degree. Such polynomial is fit on a dense grid of values

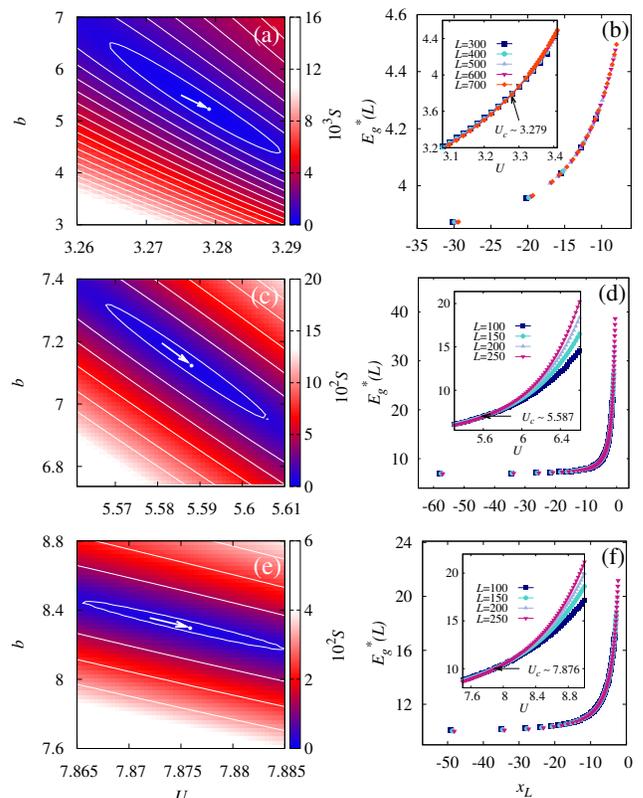


FIG. 1. (Color online) (a) Contour plot of the sum of squared residuals  $S(b, U_c)$  for  $n = 1$ . The white arrow signals the location of the minimum value of  $S$ . The white lines are equally spaced contour lines where  $S$  is constant. (b) Best collapse of the data for  $E_g^*(L)$  vs  $x_L$  corresponding to  $U_c = 3.279$ ,  $b = 5.2$ , and  $C \rightarrow \infty$ . The inset shows the rescaled gap vs.  $U$ . A similar analysis for  $n = 2$  [ $n = 3$ ] is presented in panels (c) and (d) [(e) and (f)].  $U$  and  $E_g^*$  are presented in units of  $J$ , whereas  $b$  and  $S$  are shown in units of  $J^{1/2}$  and  $J^2$ , respectively.

of  $U_c$ ,  $b$ , and  $C$ , to the calculated values of  $E_g^*(L)$  and  $x_L$ . The quality of the fit is assessed by computing the sum of squared residuals ( $S$ ), which defines the function  $S(U_c, b, C)$ .  $U_c$  is then obtained from the set of parameters  $U_c$ ,  $b$ , and  $C$  which minimizes  $S(U_c, b, C)$ . The accuracy of this method was tested by locating the critical interaction strength in a model of spinless fermions with nearest-neighbor interaction. Such a model exhibits a BKT transition for which the critical interaction strength is known analytically [18]. The value of the critical interaction strength obtained utilizing the scaling analysis of the gap described before deviates only 1% from the exact value [18], and thus we are confident that a similar or better accuracy should be attained for the BKT transition in the BHM.

We have applied this procedure to integer filled chains with  $n = 1, 2$  and  $3$ . We find that, in these three cases, the minimum of  $S(U_c, b, C)$  is obtained for arbitrarily large values of  $C$ . This means that logarithmic corrections to the scaling of the gap, in the form (2), do not

play a role in the determination of the critical point. This is to be contrasted with the  $t$ - $V$ - $V'$  model in Ref. [18], where  $C$  was found to be finite in all transitions analyzed. In Fig. 1(a), we present a density plot corresponding to  $S(U_c, b, \infty)$  for  $n = 1$ , which exhibits a clear minimum at  $U_c = 3.279 \pm 0.001$ ,  $b = 5.2 \pm 0.1$ . The error bars are estimated by repeating the minimization procedure adding and subtracting to the gap the error of the energy (overestimated to be  $\sigma_{E_g} = 10^{-6}$ ). Furthermore, the sensitivity of the results to the selection of the interval of values of  $U$  used in the fit is also included in the error bars such that our results are independent of that choice. Corresponding to the set of parameters that minimizes  $S(U, b, C)$ , in Fig. 1(b), we plot  $E_g^*(L)$  vs  $x_L$ . The data is clearly seen to collapse to a single curve representing the function  $f$ . In the inset, the curves for the rescaled gap corresponding to different system sizes are seen to merge around the critical value  $U_c$ .

Previous calculations have obtained  $U_c$  through widely different techniques, some of which we mention below. An early quantum Monte Carlo (QMC) study found  $U_c = 4.7 \pm 0.2$  using the closing of the gap at the critical point [37, 38], while later QMC simulations yielded a smaller value  $U_c = 3.33 \pm 0.06$  [39]. An approximated calculation using the Bethe ansatz suggested that  $U_c = 3.460$  [40], and strong coupling expansion calculations predicted  $U_c = 3.8 \pm 0.1$  [41]. Exact diagonalization studies led to  $U_c = 3.64 \pm 0.07$  [43], while combining exact diagonalization with renormalization group insights, a value of  $U_c = 3.28 \pm 0.02$  was reported in Ref. 42. Also, using extrapolated measurements of the fidelity susceptibility extracted from exact diagonalization of small clusters,  $U_c = 3.89 \pm 0.02$  was found in Ref. [20]. In Ref. [44], one of the first DMRG approaches to tackle this problem using extrapolations of the gap, a value of  $U_c = 3.36$  was determined. Later DMRG studies, based on accurate extrapolations of the decay of correlation functions, reported  $U_c = 3.6 \pm 0.1$  [45] and  $U_c = 3.3 \pm 0.1$  [46], and, more recently,  $U_c = 3.361 \pm 0.006$  [47] and  $U_c = 3.27 \pm 0.01$  [11]. Computing the Luttinger parameter using bipartite fluctuations, Ref. [48] reported  $U_c = 3.345 \pm 0.003$ . Finite-size scaling analyses of the von Neumann entanglement entropy suggested that  $U_c$  lays between  $U = 3.3$  and  $U = 3.4$  [49] and  $U_c = 3.27 \pm 0.03$  [50], while computations of the von Neumann entropy directly in the thermodynamic limit (using the infinite time-evolving block decimation algorithm) produced a critical value  $U_c = 3.3 \pm 0.1$  [51]. Our result for  $U_c$  is therefore in good agreement with the lowest values reported in the most recent studies that use widely diverse quantities to characterize this transition.

We have also computed the critical values for other commensurate fillings, and found  $U_c = 5.587 \pm 0.001$  for  $n = 2$  [Figs. 1(c), and 1(d)], and  $U_c = 7.876 \pm 0.002$  for  $n = 3$  [Figs. 1(e), and 1(f)]. Note that our value of  $U_c$  for  $n = 2$  is in excellent agreement with the large-scale DMRG study in Ref. [11], further supporting that the scaling of the gap utilized here is capable of providing

very accurate results at a lower computational cost. In what follows, we use our results for  $U_c$  to benchmark alternative approaches for locating the transition point.

### III. FIDELITY SUSCEPTIBILITY

The fidelity susceptibility (FS)  $\chi$  for the ground state of the system  $|\psi_0\rangle$  is defined as

$$\chi(U) = \frac{2[1 - |\langle \psi_0(U) | \psi_0(U + dU) \rangle|]}{L dU^2}, \quad (3)$$

and is also known as the fidelity metric. For generic second order phase transitions,  $\chi$  is expected to diverge in the thermodynamic limit (TL) [19, 21–23, 25], and it has been found to exhibit clear signatures of such transitions already for rather small system sizes, where a maximum of  $\chi$  was seen near the transition point [26–28, 30].

In Fig. 2, we show the fidelity susceptibility for the BHM at fillings  $n = 1, 2, 3$ , for system with  $L = 40, 80, 120$ , and for on-site interactions up to  $U = 8$ . For  $n = 1$  and  $n = 2$ ,  $\chi$  exhibits clear maxima for values of  $U$  greater than  $U_c$  computed from the scaling of the gap. Consistent with the results in Ref. [20], the positions of the maxima are seen to move towards weaker interactions, and their height to increase, with increasing system size. For  $n = 3$ , the maxima are expected to be beyond the values of  $U$  studied here. Hence, indications for the existence of a phase transition are obtained already

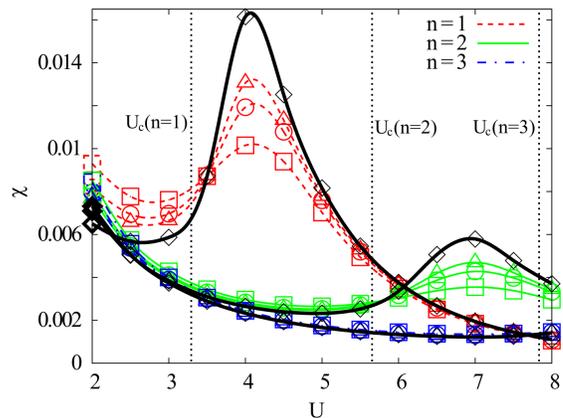


FIG. 2. (Color online) Fidelity susceptibility for different system sizes at integer filling  $n = 1$  (red symbols and dashed lines),  $n = 2$  (green symbols and solid lines) and  $n = 3$  (blue symbols and dot-dashed lines). The plot shows data for  $L = 40$  (square),  $L = 80$  (circle) and  $L = 120$  (triangle), the lines are spline interpolations and serve as a guide to the eye. The thick solid black lines (diamonds) are the result of a finite-size extrapolation using a quadratic fit. The vertical dotted lines indicate the position of the quantum critical points obtained using the scaling analysis of the gap described in the text.  $U$  and  $\chi$  are presented in units of  $J$  and  $J^{-2}$ , respectively.

for small systems. Interestingly, and also of relevance to the  $\chi$ 's calculated here, recent works have proposed that a minimum of the FS may signal the quantum critical point [29, 52]. This was argued to be possible because, depending on the scaling dimensions of the system, the FS can be finite at a critical point [21]. In Fig. 2, one can indeed see that minima of  $\chi$  also occurs close to the critical point.

It is also apparent in our results in Fig. 2 that, between the maxima and the minima, there is a point at which all values of  $\chi$  seem to be independent of  $L$  for the system sizes treated. A similar scenario was observed in the XXZ chain [24] and for SU(N) Hubbard chains [29]. As seen in Fig. 2, for  $n = 1$  and  $n = 2$ , the ‘‘crossing’’ of the FS curves for different system sizes occurs at values of  $U$  greater than  $U_c$  computed from the scaling of the gap. We applied different extrapolation schemes for  $\chi$  and did not obtain results consistent with those from the scaling of the gap: For example, in Fig. 2 we show the outcome of the simplest approach in which the extrapolation to the thermodynamic limit is attained using a second order polynomial. Neither the position of the maximum, nor the one of the minimum or of the crossing point are in agreement with the values of  $U_c$  obtained from the scaling of the gap.

As pointed out in previous studies (see, e.g., Ref. [25] for an analysis of the 1D Fermi Hubbard model), the divergence of  $\chi$  can be extremely slow and very large system sizes (as well as a more elaborate finite-size-scaling ansatz) may be required to resolve the critical point. This is further supported by the results in Ref. [24], in which a field theoretical analysis of  $\chi$  at the BKT transition in the XXZ chain unveiled a very slow divergence. However, the numerical findings for the BHM here and the XXZ chain in Ref. [24] differ in two important aspects: as opposed to the behavior of the XXZ chain, in this work we have found that logarithmic corrections are negligible in the finite size scaling of the gap of the BHM (for the system sizes analyzed). Also, the crossing point of the FS in the XXZ chain occurs for a value of the interaction strength that is smaller than the critical one, which is the opposite of what we find here for the BHM. Hence, the numerical data at hand makes it difficult to determine  $U_c$  utilizing the FS, and further studies are needed to fully understand the behavior of this quantity in the BHM, and in particular, its contrast to the one observed for the XXZ chain.

#### IV. CENTER OF MASS MOTION

In order to determine the critical point in experiments with ultracold bosons in optical lattices, we propose to follow a recent proposal that uses Bloch oscillations [31]. The idea is to apply an external field

$$V_{\text{tilt}} = -\Omega \sum_j^L j n_j, \quad (4)$$

at time  $t \geq 0$ , to a system that is initially in its ground state ( $\Omega = 0$  for  $t < 0$ ). Such a set up can be realized in optical lattice experiments by, e.g., tilting the lattice. One can then study the center of mass motion (COM)

$$x_{\text{CM}}(t) = \frac{1}{N} \sum_j^L j \langle n_j \rangle_t, \quad (5)$$

where  $N$  is the total number of particles, at times  $t \geq 0$ . In previous studies, in a variant of the  $t$ - $J$  model at low filling [31] and in an effective Ising model in a transverse field [32], it was reported that the amplitude of the COM exhibited signatures of the quantum phase transition at the critical point. In the  $t$ - $J$  like model [31], because of the formation of pairs, the transition from a metallic to a gapped superconducting phase was visible by both a rapid decrease of the amplitude and by a doubling of the frequency of the Bloch oscillations. In the Ising like model [32], the amplitude was found to be maximal at the transition point. From the experimental point of view, Bloch oscillations have been, e.g., used to investigate Dirac points on hexagonal optical lattices [53], as well as to study low-frequency breathing modes in elongated Fermi gases [54]. Here, we investigate what happens in the BHM and, at the same time, analyze the simpler (integrable) case of spinless fermions with nearest-neighbor interaction  $V$ ,

$$H = -J \sum_j (c_{j+1}^\dagger c_j + \text{H.c.}) + V \sum_j n_j n_{j+1}. \quad (6)$$

As mentioned before, this model is exactly solvable and, at half filling, exhibits a BKT transition from a Luttinger liquid (LL) to a charge density wave (CDW) insulator at  $V/J = 2$  [2, 18]. In what follows, we set  $J = 1$  and  $\hbar = 1$ , so that  $V$  is given in units of  $J$  and time  $t$  in units of  $\hbar/J$ .

In Fig. 3(a), we display the COM of a half-filled chain of spinless fermions with  $L = 20$  and different values of  $V$  on both sides of the LL to CDW transition. It is apparent that the amplitude of the oscillations decreases and the damping rate increases when increasing  $V$  and, deep in the CDW phase, no oscillations can be resolved. This is reminiscent of the behavior of a harmonic oscillator which moves freely ( $V = 0$ ), damped ( $0 < V \lesssim 2$ ) and overdamped ( $V \gtrsim 2$ ). In the LL phase, mass transport is ballistic and, therefore, it is possible for spinless fermions to freely flow upon the introduction of a small tilt of the lattice, which gives rise to COM oscillations. On the other hand, in the CDW phase the system is gapped and transport under a small tilt is suppressed, which precludes COM oscillations. A qualitatively similar behavior is observed in the COM of the BHM at filling  $n = 1$  and for  $1 \leq U \leq 5$  [Fig. 3(b)]. There, finite values of  $U \lesssim 3.5$  lead to damped oscillations, and only the first oscillation can be resolved on the time scale of our simulations. For  $U \geq 3.5$ , overdamped behavior sets in and no oscillations can be identified.

To gain a better understanding of the evolution of the Bloch oscillations as interactions are increased, in Fig. 4,

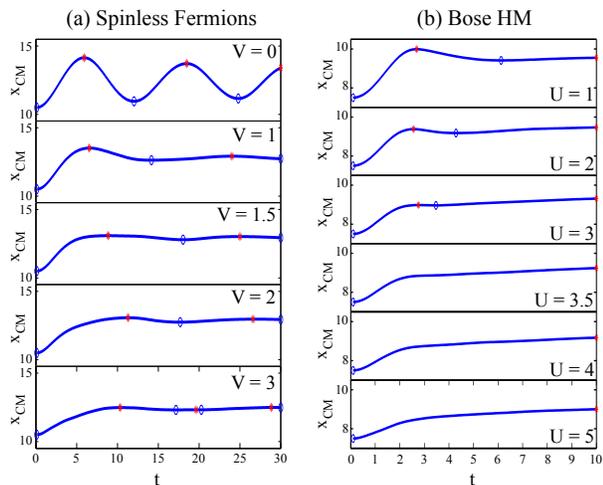


FIG. 3. (Color online) COM for (a) spinless fermions ( $L = 20$ ,  $\Omega = 1$ ) after tilting the lattice for the indicated values of  $V = 0, \dots, 3$ . (b) the BHM ( $L = 14$ ,  $\Omega = 1$ ) after tilting the lattice for the indicated values of  $U = 1, \dots, 5$ . The red stars and blue circles denote maxima and minima of the oscillations, respectively. The center of mass is presented in units of the lattice spacing  $a$ , while time  $t$  is measured in units of  $\hbar/J$ .

we display the amplitude (defined as the difference between the first maximum and the first minimum), for spinless fermions vs  $V$  [Fig. 4(a)] and for the BHM vs  $U$  [Fig. 4(b)]. For spinless fermions, it can be seen that the amplitude of the oscillations at the critical point and above ( $V \geq 2$ ) is very small and decreases with increasing system size. The results for the BHM are qualitatively similar. The region of  $U$  at which the amplitude of the Bloch oscillations is seen to vanish,  $3.0 < U \leq 3.5$ , contains the value obtained from the scaling analysis of the gap  $U_c \approx 3.279$ .

This behavior of the Bloch oscillations is also reflected in the Fourier transform (FT) of the time evolution of the COM, which we present in Fig. 4(c) for spinless fermions and in Fig. 4(d) for the BHM. In both cases, for weak interactions, there is a well defined peak around  $\omega \sim 1$ , which reflects the oscillations observed in Fig. 3. As the interaction strength is increased, the height of that peak slowly decreases and its position (slightly) changes. This is accompanied by an increase in the weight of the zero-frequency mode. For both systems, as the interaction is increased past the critical value, it is no longer possible to resolve the finite frequency peak. This is another indication that the COM oscillations are suppressed for  $U \geq U_c$ . Therefore, for both systems, the BKT transition leads to comparable behavior, and the study of Bloch oscillations in experiments can provide a good estimate of  $U_c$ .

We also studied the COM for  $n = 2$  and  $n = 3$ . Since computations become increasingly demanding with increasing filling, only smaller lattice sizes could be studied in those cases. In addition, the numerical values of the amplitude become significantly smaller.

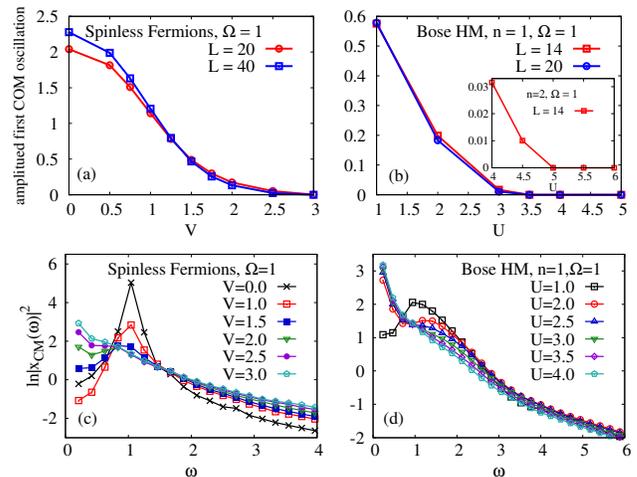


FIG. 4. (Color online) Amplitude of the first oscillation of the COM after tilting the lattice. (a) Spinless fermions at half filling ( $L = 20$  and  $L = 40$ ) and  $\Omega = 1$ . (b) BHM at filling  $n = 1$  ( $L = 14$  and  $L = 20$ ) and  $\Omega = 1$ . The inset shows results for  $L = 14$  at filling  $n = 2$ . (c) The logarithm of the amplitude square of the Fourier transform of the COM oscillations for spinless fermions at half filling with  $L = 20$  and  $\Omega = 1$ . (d) Same as in (c) but for the BHM at  $n = 1$  with  $L = 14$  and  $\Omega = 1$ . The amplitudes of COM oscillations are measured in units of  $a$ ,  $V$  and  $U$  in units of  $J$ , and  $\omega$  in units of  $J/\hbar$ .

We therefore find that theoretical estimates for  $U_c$  from the behavior of the Bloch oscillations become less accurate with increasing  $n$ . In the inset in Fig. 4(b), we show results for  $n = 2$  and  $L = 14$ , where one can see that the amplitude of the Bloch oscillations vanishes for  $4.5 < U \leq 5$ , while the theoretical prediction is  $U_c = 5.59$ . It would be interesting to study Bloch oscillations in larger lattice sizes in experiments and see if the worsening of the predictions is due to finite size effects or due to a worsening of this approach with increasing filling.

## V. CONCLUSIONS AND OUTLOOK

We followed three approaches to study quantum critical behavior in the one-dimensional BHM at integer fillings. By means of a scaling analysis of the gap, we obtained accurate values of  $U_c$  for the superfluid to Mott insulator transition at fillings  $n = 1, 2, 3$ . The fidelity susceptibility was shown to exhibit signatures of the phase transitions for finite systems, but the results for this quantity did not allow us to improve on the values of  $U_c$  obtained from the scaling of the gap. Finally, we showed that the study of Bloch oscillations in experiments can help locating the critical values for the superfluid to Mott insulator transition. The latter approach could potentially be used also in experiments in higher dimensions.

## ACKNOWLEDGMENTS

This work was supported by the Office of Naval Research and by the National Science Foundation under Grants No. PHY11-25915 and PIF-0904017, and in part

under Grant No. PHY05-25915. We thank J. Sirker, F. Gebhard, L. Campos Venuti, L. Tarruell, K. Hazzard, G. Chen, A. M. Rey, S. Ejima, and N. Bray-Ali for discussions, and acknowledge the use of computational resources at the Janus supercomputer (CU Boulder).

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