Exact diagonalization plus renormalization-group theory: Accurate method for a one-dimensional superfluid-insulator-transition study

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We use the exact-diagonalization results for a one-dimensional finite-size boson Hubbard-like Hamiltonians to initialize the renormalization-group equations in the vicinity of the superfluid-insulator transition and demonstrate that this provides a rather accurate method of extrapolation of the finite-size results to larger system sizes, and in particular, pinpointing the critical parameters of the Hamiltonians. With our approach we reproduce with the accuracy $\sim 2.5\%$ the known analytical result for the transition point in the half-filled system of hard-core bosons, obtain with a controllable accuracy the critical ratio $(t/U)_c = 0.304 \pm 0.002$ for the boson Hubbard model, and find out that, in contrast to the general belief, the reduced Hamiltonian (with the constraint that the site occupation numbers be less than 3) is far from being a good approximation to the full model.

In recent years the literature on superfluid-insulator transitions in one-dimensional (1D) systems (at $T=0$) was enlarged by exact numerical studies of finite-size Hubbard-like models based either on the quantum Monte Carlo approach[1,2] or on the diagonalization technique.[3–5] All these studies suffer one and the same generic shortcoming: dealing with the essentially finite-size systems, they are rather inaccurate in description of the transition region in the macroscopical limit, even if some extrapolation procedure is used. For one thing, the critical ratio of the hopping amplitude, t, to the on-site repulsion, U, in the boson Hubbard model with the filling factor $\nu=1$ was reported to be $(t/U)_c=0.215$ in Ref. 1 while the result of Ref. 4 is $(t/U)_c=0.275$. The cause of this shortcoming is quite clear from the universal macroscopic theory of 1D superfluid-insulator transitions[6–8]: in 1D the finite-size effects vanish logarithmically slow with increasing the size of the system. Hence, generally speaking, one would need an exponentially large cluster to observe macroscopical critical behavior. However, there is a way of overcoming this difficulty. Indeed, from the macroscopic theory it follows that the mesoscopic behavior of the system in the transition region is universal, only the particular values of the relevant parameters being unknown. Hence there arises an idea to observe this mesoscopic behavior numerically, fixing thus the unknown parameters, then to take advantage of the macroscopic theory to extrapolate the results on larger systems, and in particular on the infinite one to obtain the critical parameters of the Hamiltonian. In this paper we show how this can be done practically.

For definiteness, we consider the superfluid–Mott-insulator transition in a commensurate system. We realize, however, that our approach is applicable to the superfluid–Bose-glass transition in 1D disordered system as well.

The renormalization group equations for 1D superfluid in a commensurate potential read[8]

$$dK/d\lambda = w^2, \quad dw/d\lambda = (2-p^2/K)w. \tag{1}$$

Here $K=v/\pi\Lambda_s$, v is the sound velocity, Λ_s is the superfluid stiffness; $\lambda=\ln L$, L being a characteristic scale of distance which we will interpret as the size of the system; p is the denominator of the filling factor expressed as an irreducible fraction. While the value of $K(\lambda)$, being related to Λ_s and v is directly available from the exact-diagonalization spectra (see, e.g., Ref. 5), the value of $w(\lambda)$ can be obtained only by some recalculation. Instead of this recalculation one may take advantage of the integral of Eqs. (1):

$$Q\left(\frac{2K(\lambda_1)}{p^2}, \frac{2K(\lambda_2)}{p^2}, c\right) = 4(\lambda_2-\lambda_1),$$

$$Q(a,b,c) = \int_a^b \frac{dx}{x-\ln x - c}. \tag{2}$$

The constant c arises as a result of integrating out the variable w and is related to the particular form and parameters of the microscopic Hamiltonian. As is seen, its value is fixed once one knows the value of K at two different system sizes. To make sure that a system really obeys the universal relations (1) one may just check that the value of c is independent of the choice of λ_1 and λ_2 [up to some small finite-size corrections to Eqs. (1)]. Then, given the value of c and $K(\lambda_1)$ (λ_1 being the largest λ available numerically) one can obtain from (2) the value of K at any λ_2. Corresponding mesoscopic value of the superfluid stiffness is $\Lambda_s(\lambda_2)=v/\pi K(\lambda_2)$, the value of v being irrenormalizable.

In the superfluid phase the constant c is always less than unity, the value $c=1$ corresponding to the transition point where $K(\lambda\to\infty)=p^2/2$.[6–8] Thus to obtain the critical parameters of the Hamiltonian one should find such their combination that satisfies Eq. (2) with $c=1$. We must note here that, besides the true critical point, Eq. (2) has another (nonphysical) solution lying well inside the insulating region. It may be shown, however, that this solution occurs only at $K(\lambda_1), K(\lambda_2) > p^2/2$ and hence can be easily distinguished from the physical one.

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TABLE I. Hard-core bosons with the filling factor $\nu=1/2$.

$N_a^{(2)}/N_a^{(1)}$	$(V/t)_c$
24/22	1.937
22/20	1.927
20/18	1.914
18/16	1.898

TABLE II. Full boson model with the filling factor $\nu=1$.

$N_a^{(2)}/N_a^{(1)}$	$(t/U)_c$
12/11	0.3059
11/10	0.3062
10/9	0.3068
9/8	0.3078

Now we turn to our numerical results. We studied by Lanczos diagonalization method a few boson Hubbard models describing by the Hamiltonians of the form (either with or without a constraint on the maximum possible site occupation number)

$$H=\sum_{i=1}^{N_a}\left\{-t(e^{i\theta/N_a}a_i^+a_{i+1}+\text{ H.c.})+\frac{U}{2}n_i(n_i-1)+Vn_in_{i+1}\right\}. \tag{3}$$

Here a_i is the annihilation operator on the site i; $n_i=a_i^+a_i$. We use periodic boundary conditions and introduce the gauge phase θ, which is convenient for calculation of Λ_s by definition:

$$\Lambda_s=\lim_{\theta\to 0}2N_a[E_0(\theta)-E_0(0)]/\theta^2, \tag{4}$$

where $E_0(\theta)$ is the ground-state energy at the gauge phase θ. This way of calculating Λ_s is more accurate than that based on the supercurrent level evaluation[5] because of the splitting of the latter. With Eq. (4) and the sound velocity obtained from the one-phonon energy $E_{\text{ph}}(m)=(2\pi/N_a)vm$ one obtains $K=v/\pi\Lambda_s$ and can take advantage of Eq. (2). The most convenient choice of the momentum is $m=1$, $E_{\text{ph}}(1)=E_1-E_0$, where E_1 and E_0 are the lowest levels in the sectors of the unit and zero momenta, respectively. Note that for calculating Λ_s and v one needs only the lowest eigenvalues of the matrices, provided the numerical procedure makes use of the translational symmetry of the Hamiltonian.

First, we test our procedure on the exactly solvable model of hard-core bosons with the filling factor $\nu=1/2$. This model is described by the Hamiltonian (3) with $U\to\infty$ (or the constraint that the site occupation numbers be less than 2). This model, which at the particular filling factor $\nu=1/2$ is equivalent to the Heisenberg spin-1/2 chain, is known to undergo the superfluid-insulator transition at $V/t=2$.[9] Our aim is to reproduce this result within our approach. In Table I we present the numerical data. $N_a^{(1)}$ and $N_a^{(2)}$ are the two system sizes [$\lambda_1=\ln N_a^{(1)}$ and $\lambda_2=\ln N_a^{(2)}$], $(V/t)_c$ is the value of the ratio V/t at which Eq. (2) with $c=1$ is satisfied at given $N_a^{(1)}$ and $N_a^{(2)}$. We take $N_a^{(1)}$ as close to $N_a^{(2)}$ as possible [$N_a^{(1)}=N_a^{(2)}-2$] to minimize finite-size errors. Our data allow us to set the limits on the true macroscopic value of $(V/t)_c$. Indeed, as follows from Table I, $(V/t)_c$ as a function of $x=1/N_a^{(2)}$ has a steadily decreasing derivative as x approaches zero. Consequently, the limiting value of $(V/t)_c$ should necessarily lie between two points, one being the value corresponding to the minimal $x=x_*$, and the other being the result of the extrapolation by the straight line passing through the points corresponding to x_* and the previous one. This yields

$$(V/t)_c=1.99\pm 0.05\ \ \text{(hard-core bosons)}. \tag{5}$$

So we have reproduced the exact result with the accuracy of 2.5%. Consider now the full boson model which is described by the Hamiltonian (3) without any constraint. Since in this case the nearest-neighbor interaction does not introduce any qualitative difference, and bearing in mind comparison with the above-mentioned results of the other authors, we leave in the Hamiltonian only the on-site interaction. From the data presented in Table II we conclude that at the filling factor $\nu=1$ the transition occurs at

$$(t/U)_c=0.304\pm 0.002\ \ \text{(full boson model)}. \tag{6}$$

Note that while the maximum available system size now is two times smaller than in the case of the hard-core bosons, the relative accuracy (better than 1%) is higher.

Recently the strong-coupling expansion for Bose Hubbard model was presented.[10] The critical value of t/U for the Mott transition in 1D pure system with one particle per site (extracted from the Kosterlitz-Thouless extrapolation of the third-order results for the dielectric gap) is found to be 0.265. Although this value is noticeably greater than the non-extrapolated result $(t/U)_c=0.215$ reported earlier[11] it still differs from ours. The difference may be attributed to the fact that the curves being extrapolated in Ref. 10 are essentially approximate. In this connection note that the lower branch of the phase boundary (Fig. 1 of Ref. 10), if shifted a bit down, will fit the quantum Monte Carlo results better and will move $(t/U)_c$ towards our value Eq.(6).

The so-called reduced model differs from the full one by the constraint that the only possible site occupation numbers are zero, one, or two. There is a belief that this constraint is not so restrictive and the reduced model thus may be considered as a good approximation to the full one.[12,13] In this connection our results for the reduced model turn out to be rather unexpected: we have found that Eq. (2) with $c=1$ has no physical solution at $U\geqslant 0$, which means that the reduced model is in the insulating state everywhere in this region. In particular, in the vicinity of the transition point of the full model, $(t/U)_c\approx 0.3$, parameter K of the reduced model at our maximum numerically available $N_a=16$ is close to 0.7, i.e., the system is well inside the insulating region. The data for K as a function of the system size at $U=0$ (the most favorable point for superfluidity at $U\geqslant 0$, if any) are presented in Table III. We see that K is still a bit smaller than the critical value 0.5, but has a tendency to increase. It should be noticed, however, that the particular behavior of $K(N_a)$ at $U=0$ is rather poorly fitted by the relation (2).

TABLE III. Reduced model with the filling factor $\nu=1$ at $U=0$.

N_a	K
16	0.4523
15	0.4516
14	0.4505
13	0.4492
12	0.4477

Hence the extrapolation to larger N_a's is not so reliable. Besides, from Table III it is seen that a pronounced dielectrization (divergency of K) will occur, if any, only at very large system sizes.

It is worth mentioning the value of $(t/U)\approx 0.6$ where K at $N_a=16$ becomes greater than 0.5. This value might be considered as the lower bound for the transition point, should our extrapolation procedure turn out to be inapplicable to the reduced model for this or that reason.

Physically such a behavior of the reduced model can be understood if one takes into account that the requirement having at most double occupancy plays a role of specific repulsive interaction which turns out to be rather strong, in contrast to what one could expect.

A discussion of Ref. 12 is in order here. In this reference the Bethe-ansatz (BA) for 1D boson Hubbard model was studied, and it was shown that despite the fact that BA is not an exact method for this problem it yields an excellent approximation to the results obtained by quantum Monte Carlo simulations. [The only inconsistency of BA is a divergency of the superfluid density in a close vicinity of the critical point.] Note also that the BA value $(t/U)_c=1/2\sqrt{3}\approx 0.289$ (Ref. 12) is very close to ours. The success of BA for the full boson Hubbard model was attributed to the small probability to find a multiply (i.e., more than doubly) occupied site. Moreover, it was claimed that if this probability were zero, BA approximation would be exact. Clearly, this particular assertion is in a sharp disagreement with our results on the reduced model: in this case there are no multiply occupied sites by definition, but instead of observing a perfect correspondence with the BA results of Ref. 12 we see a dramatic change in the properties of the system.

We have also considered the model with the constraint $n_i<4$ at $\nu=1$. In contrast to the model $n_i<3$, we found the critical properties of this system to be very close to these of the full model. In particular, for the transition point we obtained $(t/U)_c=0.313\pm 0.003$. The value of K at $U=0$ [to be compared to the model $n_i<3$] is ≈ 0.20.

In conclusion, we have presented a method which yields a regular solution to the known 1D problem of logarithmically slow convergence of the finite-size results towards the thermodynamic limit in the vicinity of the transition points, and in particular allows pinpointing the critical parameters of the Hamiltonians with a few percent accuracy. Upon a successful testing of the method on the exactly solvable half-filled hard-core boson Hubbard model we have used it to find the critical point of the commensurate (one particle per site) boson Hubbard Hamiltonian, where previously reported results demonstrate a considerable discrepancy with each other. Our result (obtained with less than 1% accuracy) turns out to be very close (within $\sim 3\%$) to the Bethe-ansatz approximation,[12] not far ($\sim 10\%$) from those of Refs. 4,10, and differs noticeably ($\sim 30\%$) from the result of Ref. 1.

We have also observed an unexpectedly important role of triply occupied sites in the commensurate boson Hubbard model: a constraint prohibiting more than doubly occupied sites changes dramatically the long-range properties of the system and can even destroy superfluidity at any value of the on-site repulsion.

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