Phase Transitions in One-Dimensional Truncated Bosonic Hubbard Model and Its Spin-1 Analog

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We study one-dimensional truncated (no more than 2 particles on a site) bosonic Hubbard model in both repulsive and attractive regimes by exact diagonalization and exact worldline Monte Carlo simulation. In the commensurate case (one particle per site) we demonstrate that the point of Mott-insulator – superfluid transition, $(U/t)_c = 0.50 \pm 0.05$, is remarkably far from that of the full model. In the attractive region we observe the phase transition from one-particle superfluid to two-particle one. The pairing gap demonstrates a linear behavior in the vicinity of the critical point. The critical state features marginal response to the gauge phase. We argue that the two-particle superfluid is a macroscopic analog of a peculiar phase observed earlier in a spin-1 model with axial anisotropy.

I. INTRODUCTION

In the family of Hamiltonians, which the physics of strongly correlated systems deals with, the one-dimensional bosonic Hubbard one,

$$H = \sum_{i=1}^{N} \left\{ -t (a_i^\dagger a_{i+1} + H.c.) + \frac{U}{2} n_i (n_i - 1) \right\},$$

$[a_i^\dagger]$ creates a particle on the site $i$, $t$ is the hopping amplitude, $n_i = a_i^\dagger a_i$, $N$ is the number of sites] plays an important part as a laconic model for the superfluid (SF) – Mott-insulator (MI) phase transition (and for SF – Bose-glass (BG) and BG–MI transitions in the presence of disorder). Along with the full model Eq. (1.1) sometimes actually its truncated counterpart, defined by the requirement that site occupation numbers are less than 3, is considered: either deliberately, for the purpose of simplification, or implicitly, in approximate treatments which do not distinguish between the full and the truncated models. One ordinarily motivates such a replacement by the observation that in the full model even at the boundary point $U = 0$ [At $U < 0$ the system is unstable against a collapse of almost all the particles onto one site.] the quantum-mechanical probability to find out that the occupation number of a given site is greater than 2 equals to $(e - 5/2)/e \approx 0.080$, so it is very likely that the tripoly (and more) occupied sites play no essential role.

However, a rather accurate method “exact diagonalization plus renormalization group (RG)” demonstrated the absence of the superfluid phase in the truncated model almost down to $U = 0$, in sharp contrast to the above-mentioned reasoning, and to the results of a number of approximate treatments. It is essential that the conclusion of Ref. demonstrated the absence of superfluidity in the macroscopic limit is not a direct one. What was really demonstrated is that at arbitrarily small $U$ the known RG flow of superfluid parameters, initialized numerically at intermediate scales, leads to the destruction of superfluidity in favor of Mott insulator. Hence, it would be instructive to check this fact explicitly by Monte Carlo (MC) simulation of a sufficiently large system, allowing direct measuring the insulating gap at $U \ll 1$. This is the primary goal of the present paper.

Another interesting aspect of the truncated bosonic Hubbard model, distinguishing it from the full one, is that at $U < 0$ it is stable against the collapse onto one site. Therefore our secondary goal is to investigate the region of attraction: First, one may expect to find here the superfluid phase. Secondly, at a sufficiently strong attraction a pairing of particles should take place, as is clear from the perturbative analysis at $U \rightarrow -\infty$, and it is interesting to study numerically the corresponding phase transition. Note that in Ref. the close problem of the BCS-like pairing was examined in a dilute atomic Bose gas with an effective attractive interaction.

Finally, 1D truncated bosonic Hubbard model is not of academic interest only. Macroscopically, it is very close to a spin-1 (anisotropic) chain in an easy-axis ($U < 0$), or easy-plane ($U > 0$) environment. Its study thus provides deep insight into the physics of phase transitions in the spin chains.

In the present paper we report a study of the model by the exact continuous-time worldline MC approach, developed recently by Prokof’ev, Svistunov and Tupitsyn. (Some preliminary results were obtained by the standard worldline
MC method. For some special purposes we also employ exact diagonalization.) In the commensurate case we have found the critical value of the MI–SF transition, \((U/t)_c = 0.50 \pm 0.05\), which is more than 6 times lower than that of the full model. In the attractive region, \(U < 0\), we observe a specific pairing phase transition when the system passes from the one-particle superfluid vacuum to the two-particle one. At the filling factor equal to unity [commensurability being not relevant] the transition occurs at \(U/t \approx -6.0\). The critical behavior is characterized by linear collapse of the pairing gap as a function of \(U\), and by a marginal response to the gauge phase at the transition point.

We also consider spin-1 analog of the truncated bosonic model, which was studied earlier by exact diagonalization.\(^{13}\) The question of our interest here is a peculiar phase which was observed in Ref. 8, but was not revealed in Ref. 13, and, as far as we know, was never discussed since then. We demonstrate that the phase does really exist, being a direct macroscopic analog of the two-particle superfluid phase of the bosonic system.

### II. REPULSIVE REGIME

The MI–SF transition in the truncated one-dimensional commensurate bosonic Hubbard model was studied previously by a number of approximate methods. In Ref. 6 the real-space renormalization-group method was used, with the result \((t/U)_c = 0.215\) for the critical point. In Ref. 7 Bethe-ansatz approximation for the full model was considered, with a conjecture that the approximation actually corresponds to the exact solution of the truncated model. The critical value obtained was \((t/U)_c = 0.289\). In Ref. 8 the strong-coupling expansion for the full model was examined. The results \((t/U)_c = 0.215\) for the bare third-order expansion, and \((t/U)_c = 0.265\) with a correction to the Kosterlitz-Thouless critical behavior are quite applicable to the truncated model, since the triply and more occupied sites contribute only to the higher-order terms.

The above-cited results are more or less close to each other, and to the critical value of the full model, \((t/U)_c = 0.304 \pm 0.002\), obtained with a controllable accuracy by an accurate method “exact diagonalization + renormalization-group (RG) analysis.”\(^ {15}\) Practically the same value, \((t/U)_c = 0.30\), was found also by density-matrix real-space RG methods\(^ {11}\) and by accurate MC simulations.\(^ {16}\) However, the method of Ref. 8 demonstrated that in the truncated model the critical value should be essentially shifted towards small \(U\)’s: at \(t/U = 0.3\) the truncated system was found well inside the insulating region. Moreover, the very fact of the existence of superfluidity at \(U > 0\) was questioned [with a reservation that the maximal available size of the cluster, 16 sites, was not enough to resolve unambiguously the behavior at small \(U\)’s.]

To clarify this situation, we perform an accurate MC study of the commensurate truncated model. We start with the standard worldline MC method\(^ {11}\) and the standard calculation of the insulating gap \(\Delta = \mu_+ - \mu_-\), where the chemical potentials \(\mu_+\) and \(\mu_-\) are given by the relations \(\mu_+ = E(N_a + 1) - E(N_a)\) and \(\mu_- = E(N_a) - E(N_a - 1)\), \(E(N)\) being the energy of a system consisting of \(N\) bosons. In \(\mu_\pm vs t/U\) diagram the region of the insulator phase is bounded by the curves \(\mu_+(t/U)\) and \(\mu_-(t/U)\). This diagram for \(N_a = N_b = 50\) is shown in Fig. 1, in comparison with that for the full system. At large \(U/t\) phase boundaries in the truncated case are close to those of the full one. This is the region, where the strong-coupling approximation is rather accurate. At smaller \(U/t\), however, the difference between the full and truncated models is clearly seen. At \(U/t < 3.3\), where the full model is already in the superfluid phase, the truncated model demonstrates a small, but quite pronounced insulating gap. It is seen also, that the system is rather subtle in this region, as the gap is considerably smaller than the hopping amplitude. This feature makes it difficult to extract the critical point from the data presented, even with the RG-analysis of the gap, since the computational errors (\(~ 0.05t\) are comparable with the typical values of the gap (\(~ 0.1t\)) in a rather extensive critical region.

Fortunately, for the problem of pinpointing the critical ratio \(U/t\) we had an opportunity to take advantage of the continuous-time worldline MC approach with “worm” update.\(^ {12}\) The code described in Ref. 11 directly applies to our problem. Working in the grand canonical ensemble, the code allows to extract the macroscopic parameter \(K\) (main superfluid characteristic of one-dimensional system) from the histograms for winding numbers and numbers of particles.\(^ {11}\) Given the values of \(K\) for two different system sizes, one easily obtains macroscopic value of \(K\) from the first integral of the RG equations, and is able thus to determine whether the system is superfluid or dielectric in the macroscopic limit.\(^ {11}\) The sizes of the systems we used for this purpose were \(N_a = 128\) and \(N_a = 16\). This way we obtained the critical point of the SF–MI transition in the truncated model. (The details of calculation and the estimation of the error see in Ref. 11)

\[
(U/t)_c = 0.50 \pm 0.05
\]  

As expected, this critical ratio is several times lower than that of the full model.
III. ATTRACTIVE REGIME

Consider the truncated model with the attractive interaction, \( U < 0 \). The behavior of the truncated model in this region differs qualitatively from that of the full one, the latter being just trivial because of the collapse of almost all of the particles onto one site. The constraint on the occupation numbers renders the truncated model stable against the collapse, so the point \( U = 0 \) is not a special one for it.

In Fig. 2 we show the \( \mu \) vs \( U/t \) diagram for the truncated model in the wide range of variation of \( U/t \), including the attractive region up to \( |U|/t = 8 \). In the region \(-6.0 < U/t < 0.5\) the one-particle gap vanishes, indicating that the ground state is an ordinary one-particle superfluid. At \( U/t < -6.0 \) the one-particle gap (\( \Delta \sim |U| \)) appears again. Apparently, the point \( U/t < -6.0 \) corresponds to the pairing of the carriers. To demonstrate the liquid behavior of the two-particle state, we calculate two-particle gap \( \Delta_2 = \mu_{2+} - \mu_{2-} = E(N_b + 2) - E(N_b) \), \( \mu_{2-} = E(N_b) - E(N_b - 2) \). The results are presented in Fig. 3. These reveal the gap corresponding to one-particle Mott insulator at \( U/t > 0.5 \), and absence of the gap at negative \( U \)’s.

In Fig. 4b we show the one-particle gap at the critical region. Within the accuracy of our results, the gap varies linearly with \( U/t \).

Obviously, the pairing transition, being of liquid-liquid type, should take place for non-commensurate fillings as well. [We checked this explicitly for certain non-commensurate fillings.] Though not relevant for the pairing transition, commensurability may lead however to the formation of the Mott insulator for pairs. The absence of the two-particle well. [We checked this explicitly for certain non-commensurate fillings.]

IV. RESPONSE TO GAUGE PHASE

Pairing leads to a dramatic change in the response of the system to the global gauge phase. It is instructive thus to study this response in the vicinity of the critical point.

We introduce the gauge phase, \( \Phi \), to the model by conventional transformation of the hopping amplitude: \( t \to t \exp(i\Phi/N_a) \).

First we study the groundstate energy, \( E_0 \), as a function of \( \Phi \), at different \( U \)’s, by exact diagonalization for the chain \( N_a = N_b = 12 \), see Fig. 5. [The results for the groundstate persistent current, \( J_0(\Phi) \), immediately follow from \( J_0(\Phi) = dE_0(\Phi)/d\Phi \).] Curve 1 corresponds to the well-defined one-particle ground state laying in the zero momentum sector at any value of \( \Phi \). The well-defined two-particle ground state (curve 4) lays in the zero sector while \( \Phi \) varies from 0 to \( \pi/2 \). At \( \Phi = \pi/2 \) it jumps to the momentum sector \( N_b/2 \) (in the units of minimal non-zero momentum), and remains there till \( \Phi = 3\pi/2 \). The curve \( E_0(\Phi) \) acquires a characteristic cusp form, symmetric with respect to the line \( \Phi = \pi/2 \). Curves 2 and 3, corresponding to the cross-over region, demonstrate a marginal behavior of \( E_0(\Phi) \): The ground state lays in the zero momentum sector until the phase reaches some critical value (greater than \( \pi/2 \)), and then jumps to the sector \( N_b/2 \). The curve is not symmetric with respect to the cusp point.

We see that the marginal response to the gauge phase in the vicinity of the critical point is due to the competition (at \( \Phi > \pi/2 \)) between the groundstate in zero sector and that in the sector \( N_b/2 \). At finite, but sufficiently low temperatures both states contribute to the marginal response (provided the system is close enough to the critical point), with their Gibbs factors. As an example, we present in Fig. 6 the equilibrium persistent current as a function of \( \Phi \) obtained by MC.

The marginal response to the gauge phase can be used to obtain a rather accurate extrapolation for the critical point. At \( N_a \to \infty \) the size of the cross-over region, where the marginal response takes place, tends to zero. Hence, we may consider the value of \( U \), corresponding to some characteristic marginal-response feature, as a function of

\[
H_{\text{eff}} = \frac{t^2}{U} \sum_{i=1}^{N_a} \left\{ -b_i^{\dagger} b_{i+1} + \text{H.c.} \right\} + 2 \sum_{i=1}^{N_a} \left( b_i^{\dagger} b_{i+1}^{\dagger} b_{i+1} b_i \right),
\]

(3.1)

where \( b_i^{\dagger} \) creates a pair on the site \( i \). The states with single occupations of sites are separated from the ground state by the gap close to \( |U| \). We thus come to the familiar 1D half-filled hard-core model with the parameters corresponding just to the critical point of superfluid - insulator (commensurate density wave) transition (see, e.g., [8]). So we conclude that in our model the “critical point” for the Mott transition for pairs is \( U = \infty \), and for finite \( U \)’s the transition does not take place.
and extrapolate to $N_a = \infty$. For one thing, one may consider just the point of the appearance of the marginal response, i.e. the point where at the phase $\Phi = \pi$ the energies in the zero sector and in the sector $N_b/2$ coincide. Corresponding extrapolation from the exact-diagonalization results is presented in Fig. 7. The difference between the results of linear and quadratic extrapolations provides a reasonable estimate for the error.

V. SPIN-1 CHAIN WITH AXIAL ANISOTROPY

Macroscopically, the truncated bosonic model considered (TBM) in the previous sections is analogous to the spin-1 chain with axial anisotropy (S1):

$$H = -\frac{t}{2} \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + V \sum_{\langle ij \rangle} S_i^z S_j^z + U \sum_i (S_i^z)^2,$$  (5.1)

where $U$ is the parameter of the interaction with the easy-magnetization axis, if $U < 0$, or easy-magnetization plane, if $U > 0$. Generally speaking, the term with $V$ renders the model (5.1) much richer than the model (1.1). Obviously, to make the analogy more close, one should also add a term with nearest-neighbor interaction to the Hamiltonian (1.1). To our purposes, however, this is not essential.

The zero-point phase diagram of the model (5.1) was studied in Refs. 12, 13 by exact diagonalization on the chains up to $N_a = 12$, see Fig. 8. The phases were identified as follows:

1) ferromagnetic ($\langle S^z \rangle = \pm N_a$);
2) antiferromagnetic ($\langle S^z \rangle = 0$ in the ground state as well as in the first excited one);
3) Haldane gap state (the state with the gap in the spectrum, and $\langle S_2^z \rangle = \pm 1$ in the first excited state);
4) XY-spin liquid (the gapless state with $\langle S_2^z \rangle = \pm 1$ in the first excited state).

[Haldane gap state in S1 is equivalent to Mott state in the TBM, while the XY-spin liquid in S1 is equivalent to one-particle superfluid in the TBM.]

Besides, in Ref. 12, one more phase was observed, the so-called “spin-1/2-like XY-phase” (region 5 in Fig. 8), which was characterized by $\langle S_2^z \rangle = 0$ in the ground state and $\langle S_2^z \rangle = \pm 2$ in the first excited state. But later, in Ref. 13, this phase was not detected, and, as far as we know, it had not been mentioned in literature since that time.

Our aim is to make sure that this phase does really exist and is equivalent to the two-particle superfluid in TBM. To this end we perform MC simulation of the model (5.1) in the bosonic representation (Holstein-Primakoff transformation) for $N_a = 50$, at $V = -0.05t$. The $\mu$ vs $U/t$ diagram is shown in Fig. 9. It demonstrates the remarkable similarity with the behavior of TBM near the point of the pairing phase transition: the one-particle gap, which shrinks linearly in the wide interval of the parameter $U$. The critical point $(U/t)_c \approx -2.0$ coincides with the value found in Ref. 14.

Note that in the limit $U \rightarrow \infty$ the model (5.1) with $V = 0$ also approaches the effective Hamiltonian (3.1), and the equivalence to TBM becomes exact.

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FIGURE CAPTIONS

Fig. 1. $\mu$ vs $U/t$ diagram for the truncated model ($\circ$) with $N_a = N_b = 50$ obtained by the Monte Carlo method. $T = 0.0625t$. For comparison the phase diagram of the full boson model (+) is shown.

Fig. 2. $\mu$ vs $U/t$ diagram, obtained for $N_a = N_b = 50$ by Monte Carlo in the wide parameter region.

Fig. 3. $\mu_2$ vs $U/t$ diagram for $N_a = N_b = 14$ (exact diagonalization).

Fig. 4. One-particle gap at the critical region $T = t/50$, $N_a = 50$ (Monte Carlo).

Fig. 5. Groundstate energy vs gauge phase at $N_a = N_b = 12$ (exact diagonalization): (1) $U/t = -5.5$, (2) $U/t = -6.0$, (3) $U/t = -6.5$, (4) $U/t = -10.0$.

Fig. 6. Equilibrium persistent current vs gauge phase in the marginal region. $U/t = -5.92$, $N_a = 50$, $T = t/150$.

Fig. 7. Scaling for the point of the appearance of the marginal response to the gauge phase for chains with $N_a = 8, 10, 12, 14, 16$ (exact diagonalization).

Fig. 8. Phase diagram for spin-1 chain with axial anisotropy, from Ref. 12. (1) ferromagnetic state, (2) antiferromagnetic state, (3) Haldane gap state, (4) $XY$-spin liquid, (5) “spin-1/2-like $XY$-phase”.

Fig. 9. $\mu$ vs $U/t$ diagram for the spin chain. $V/t = -0.05$, $N_a = 50$, $T = t/50$.

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\( (E(\phi) - E(0))N_\alpha \) vs \( \phi/\pi \)
