Density matrix renormalization group for disordered bosons in one dimension

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We calculate the zero-temperature phase diagram of the disordered Bose-Hubbard model in one dimension using the density matrix renormalization group. For integer filling the Mott insulating state are always separated by a Bose glass phase as suggested by Fisher et al. The superfluid density is nonmonotonic not only as a function of interaction but also of disorder. Thus for strong repulsion increasing disorder drives a transition from a Bose glass to a superfluid. For half filling, where no Mott insulator exists, the superfluid density is again a nonmonotonic function of the repulsive interaction, however disorder now always suppresses superfluidity as expected. The corresponding phase diagram is in agreement with that suggested by Giamarchi and Schulz

The Bose-Hubbard model in 1d is defined by the Hamiltonian

\[ H = -t \sum_i (b_i^\dagger b_{i+1} + h.c.) + U \sum_i n_i(n_i - 1) + \sum_i \epsilon_i n_i. \]

(1)

Here \( b_i^\dagger \) is the boson creation operator on site \( i \) of a 1d lattice with \( L \) sites and \( n_i = b_i^\dagger b_i \) the corresponding local occupation number with eigenvalues 0, 1, 2, \ldots. The kinetic energy is described by a hopping matrix element \( t > 0 \), leading to a standard tight binding band \( \epsilon(k) = -t \cos k \) in the presence of interactions and randomness. The repulsive interaction is described by a local, positive Hubbard \( U \) which increases the energy if more than one boson occupies a given site. Finally the site energies \( \epsilon_i \) are assumed to be independent random variables with zero average and a box distribution in the interval from \( -\Delta \) to \( \Delta \). Throughout we work in the canonical ensemble with a given (dimensionless) density \( n = \frac{N}{L} \) of bosons. As usual we choose \( t = 1 \) as a unit of energy (note that some authors have \( t \) instead of \( \frac{1}{2} t \) in the hopping or 2\( \epsilon_i \) in the site energies which leads to a trivial factor of two difference with our results). Apart from the density \( n \), this leaves the two dimensionless parameters \( U \) and \( \Delta \) characterizing the interactions and disorder which completely specify the problem at zero temperature. In order to distinguish the various possible phases, we calculate both the energy gap \( E_g \) and the superfluid fraction \( \rho_s \).
energy gap which is only nonzero in a Mott insulating phase, can either be evaluated directly from a numerical calculation of the energy of the ground and first excited state. Alternatively the gap can be obtained as the difference $E_0 = \mu_p - \mu_n$ between the chemical potential for particle ($\mu_p = E_{N+1} - E_N$) or hole excitations ($\mu_n = E_N - E_{N-1}$). We have employed both methods in order to check our results. For the superfluid fraction $\rho_s$, we use the thermodynamic definition proposed by Fisher, Barber and Jasnow. It is based on defining $\rho_s$ via the sensitivity to a change in the boundary conditions between periodic (pbc) and antiperiodic (apbc) ones. In one dimension, at a given density $n = \frac{N}{L}$, the superfluid fraction $\rho_s$ is thus given by (at $t = 1$)

$$\rho_s = \frac{2L}{\pi^2} \frac{L}{N} \left[ E_0^{\text{apbc}}(L) - E_0^{\text{pbc}}(L) \right]$$

where $E_0(L)$ are the ground state energies for the specific boundary condition. In the absence of interactions and disorder it is straightforward to show that $\rho_s = 1$ for arbitrary densities $n$ as it should be. It is important to note that it is precisely a nonvanishing value of $\rho_s$ (in the limit $L \to \infty$) which is the relevant criterion for superfluidity despite the fact that the one particle density matrix $(b_i^\dagger b_i)$ decays to zero algebraically, i.e. only exhibits quasi-long range order.

For the numerical calculations it is obviously necessary to limit the number of bosons which can occupy a given site. In order to be able to cover also small values of $U$, where many bosons tend to cluster at locally favorable sites, we have truncated our basis to $m = 7$ states for each site $i$ which allows up to 6 bosons occupying the same place. We have checked carefully that our results do not depend on $m$, which was the case at least down to $U \approx 0.5$. In the DMRG calculation we studied system lengths up to $L = 50$ and included up to $M = 190$ states. For the truncation error, which is one minus the density matrix eigenvalues $\lambda_\alpha$ of all $M$ states kept in the decimation,

$$\rho = 1 - \sum_{\alpha=1}^M \lambda_\alpha,$$

we find values of the order of $10^{-10}$. A very important point which turns out to be absolutely crucial for applying the DMRG to disordered systems is to apply the finite size (“sweeping”) algorithm. After the system has been grown to its full length, renormalization group transformations have not yet been able to take into account the full structure of disorder while working on shorter systems. The finite size algorithm then works on the complete system, and improves results essentially in a variational fashion. We find good convergence of both the gap and the superfluid fraction after several sweeps. The dependence on the number of states kept was comparatively weak (also compared to the scattering of results in various realisations of disorder) such that we preferred to invest computational resources rather in sweeps. The antiperiodic boundary condition has been implemented by replacing the hopping energy $t$ at one of the bonds by $-t$ thus enforcing a localized twist in the phase by $\pi$.

![FIG. 1. Phase diagram for commensurate filling $n = 1$. Error bars are mainly due to the dependence of results on the realisations of disorder. Above a disorder strength $\Delta_{\text{max}} = 4$ it is always energetically advantageous to destroy superfluidity in favor of a glass phase.](image)

For the discussion of our results we first concentrate on a commensurable density $n = 1$, where a Mott insulating phase is expected at sufficiently large $U$. In the limit of vanishing disorder $\Delta = 0$ the system is superfluid at small values of $U$ with a superfluid fraction $\rho_s$ which monotonically decreases from one at $U = 0$ to zero at $U = U_c$. Since the transition to the Mott insulator is driven by phase fluctuations at a given density, it is a Kosterlitz-Thouless like transition very similar to the one present in a chain of Josephson junctions with a local charging energy. Our numerical result for the critical value of $U$ is $U_c(\Delta = 0) = 1.92 \pm 0.04$ which is surprisingly close to that found in mean field theory. It also agrees with a very recent DMRG calculation of the Bose-Hubbard model without disorder by Kühlner und Monien. They have used the condition that the exponent $K$ characterizing the decay of the off-diagonal density matrix

$$\langle b_i^\dagger b_j^\dagger \rangle \sim |i|^{-K/2}$$

in the superfluid phase takes on the value $K_c = 1/2$ at the transition. Note that $K$ scales like $\sqrt{U/t}$ at least in a Josephson junction array description which is equivalent to the Bose-Hubbard model at large integer densities. At finite disorder the Mott insulating phase is suppressed because the energy gap is reduced. For vanishing hopping, i.e. $U \to \infty$ effectively, the reduction is just $2\Delta$. Thus in the limit of large $U$ the Mott-insulator disappears of $\Delta > U/2$. This is in fact the asymptotic behaviour of
the transition line shown in Fig. 1. For nonzero $t$, i.e. finite $U$ the transition appears earlier, until the Mott insulator completely disappears at $U < U_c(\Delta = 0) = 1.92$. Outside the Mott-insulating phase the gap vanishes, however at finite disorder the system need not be superfluid. Indeed calculating the superfluid fraction $\rho_s$, we find that $\rho_s$ is nonvanishing only in the superfluid regime in Fig. 1, which bends down to $\Delta = 0$ both near $U = 0$ and $U = U_c(\Delta = 0)$. As a consequence, at finite disorder, there is no direct transition from a Mott insulator to a superfluid in agreement with the arguments given by Fisher et al. and Freericks and Monien. The complete phase diagram is shown in Fig. 1. It agrees well with that found by Prokof'ev and Svistunov using a rather different method and also with the qualitative picture put forward by Herbut. By contrast, there are strong, even qualitative differences with the phase diagram found by Pai et al. Their failure to see the intervening Bose-glass between the superfluid and the Mott-insulator is probably related to the fact that without the sweeping algorithm the treatment of a disordered problem by the DMRG is not reliable. Regarding the general structure of the phase diagram shown in Fig. 1, we expect that it will not be qualitatively different for the two dimensional case (though the corresponding path integral Monte Carlo calculations of Krauth, Trivedi and Ceperley and also more recent ones failed to see the intermediate Bose-glass between the superfluid and the Mott-insulator). Assuming that the phase diagram of Fig. 1 is indeed generic for the disordered Bose-Hubbard model at commensurate densities, one can draw two general conclusions:

(i) Since the superfluid fraction is a nonmonotonic function of $U$ for a given disorder, repulsive interactions have a delocalizing tendency at small $U$ but enhance localization at large $U$. This is in fact a general property, valid also at incommensurate densities as verified by Scalettar, Batrouni and Zimanyi for $n = 0.625$ and our own results at $n = 0.5$.

(ii) More surprisingly, for fixed repulsion in the range $U > U_c(\Delta = 0)$ but not too large, increasing disorder drives a Bose-glass to superfluid transition. Thus increasing disorder may in fact favour superfluidity (see dash-dotted line in Fig. 1). The associated superfluid fraction is finite only for $\Delta > \Delta_c(U)$. It first increases with $\Delta$ but eventually decreases to zero again at the upper boundary $\Delta_c(U)$. This effect may be understood by observing that with increasing distance from the Mott insulator the density of mobile particle-hole excitations increases, thus enhancing $\rho_s$. At larger values of $\Delta$ the disorder induced localization takes over and $\rho_s$ goes to zero again at the upper phase boundary $\Delta_c(U)$.

For the study of a noncommensurate density, we have chosen $n = 0.5$ where the Mott-insulating density is completely absent. The resulting phase diagram is shown in Fig. 2. It exhibits a superfluid phase in a finite regime $U - (\Delta) < U < U_c(\Delta)$ of the repulsion provided the disorder is below a critical value $\Delta_{max} \approx 0.95$. The error bars in the determination of the phase boundary are larger than in the case $n = 1$ because the superfluid fraction exhibits rather strong realization dependent fluctuations. This problem becomes particularly relevant in the limit of small $U$. In fact noninteracting bosons are a singular limit of the disordered Bose-Hubbard model since particles will collapse into the single level with the lowest $\epsilon_i$, which will vary between different realizations. For small but finite $U$ the ground state densities are still rather nonuniform. Now on the basis of that, it has been conjectured by Scalettar et al. that there are two qualitatively different localized states, a suggestion originally due to Giamarchi and Schulz. The two phases would be separated by a line $\Delta_c(U)$ above $\Delta_{max}$ which meets the phase boundary to the superfluid at a multicritical point. In order to look for signatures of this boundary at $\Delta > \Delta_{max}$, we have calculated the expectation value of the dimensionless disorder energy per particle

$$S = \frac{1}{\Delta N} \sum_i \epsilon_i \langle n_i \rangle,$$  

(5)

which is finite for a localized state. Although $S$ becomes increasingly negative as $U$ is lowered, approaching the limit $S = -1$ at $U \ll 1$, we have found no indication of any abrupt changes. This suggests that there is no quantitative distinction between an “Anderson glass”
for small $U$ and a Bose-glass for larger repulsion. Verly likely it is only the line $U = 0$ which is singular. This point of view is supported further by the fact that the phase diagram found by Prokof’ev and Svistunov[12] on the basis of the Giamarchi and Schulz criterion[13] $K_c = 2/3$ for the renormalized exponent in the decay of the off-diagonal density matrix (4) essentially coincides with our results. Thus for any point on the phase boundary between the superfluid and the Bose-glass, scaling is towards $\Delta = 0$, $K = 2/3$ even for very small $U$. Finally we have also determined the superfluid fraction as a function of $U$, which exhibits a maximum at $U \approx 1 - 1.5$. Unlike the case for $n = 1$ this maximum does not scale to larger $U$ if $\Delta$ is increased. For very small $\Delta$ the critical value $U_c(\Delta = 0) = 3.2(2)$ beyond which $\rho_s$ vanishes in the presence of even a very small randomness has been determined by calculating the exponent $K$ in the pure system and using the criterion $K_c = 2/3$. Quite generally, however, the numerical calculation of $\rho_s$ becomes rather difficult for small disorder. This is probably related to the strong divergence $\xi \sim (\frac{1}{\Delta})^{1/(3-2/K)}$ of the localization length in the limit $\Delta \to 0$ near the critical point $K_c = 2/3$, which follows from the integration of the Giamarchi and Schulz flow equations. For vanishing disorder $\rho_s$ is finite for arbitrary values of $U$, approaching $\rho_s = 2/\pi$ as $U \to \infty$ where the Bose-Hubbard model at $n = \frac{1}{2}$ is equivalent to the exactly soluble quantum XY-model in zero magnetic field. Since $K = \infty$ in this limit, the localisation length in the XY-model with a random local field is expected to diverge like $(\frac{1}{\Delta})^{1/3}$.

In conclusion we have demonstrated that the DMRG method can be successfully applied to systems with quenched disorder. The phase diagram of the 1d Bose-Hubbard model has been determined both at integer and at half filling. It exhibits significant differences with earlier DMRG results[11] but essentially agrees with a very recent quantum Monte Carlo calculation[10]. Our conclusions quantitatively support the general picture for the disordered Bose-Hubbard model developed by Giamarchi and Schulz[13] and by Fisher et al.[12]. The model studied here is probably the simplest example for the interplay between interactions and disorder and as such is clearly of interest in itself. Experimental realisations e.g. in terms of vertices in a 1d array of Josephson junctions with disorder[14] or the recent suggestion that Bose-Hubbard physics may be relevant for cold atoms in optical lattices[15] will certainly further the interest in this model.

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