Destruction of diagonal and off-diagonal long range order by disorder in two-dimensional hard core boson systems

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We use quantum Monte Carlo simulations to study the effect of disorder, in the form of a disordered chemical potential, on the phase diagram of the hard core bosonic Hubbard model in two dimensions. We find numerical evidence that in two dimensions, no matter how weak the disorder, it will always destroy the long range density wave order (checkerboard solid) present at half filling and strong nearest neighbor repulsion and replace it with a Bose glass phase. We study the properties of this glassy phase including the superfluid density, energy gaps and the full Green’s function. We also study the possibility of other localized phases at weak nearest neighbor repulsion, i.e. Anderson localization. We find that such a phase does not truly exist: The disorder must exceed a threshold before the bosons (at weak nn repulsion) are localized. The phase diagram for hard core bosons with disorder cannot be obtained easily from the soft core phase diagram discussed in the literature.

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I. INTRODUCTION

The two dimensional bosonic Hubbard model has been the subject of intense interest these past years because it is thought to capture many of the important qualitative features of two dimensional superconductors and superfluids at very low temperature. For example, Helium atoms adsorbed on a surface can clearly be described by bosons moving in a two dimensional environment. It is then natural to examine the role of disorder in localizing the bosons and producing exotic phases such as a Bose glass or a normal fluid at zero temperature. In the case of soft core bosons with contact repulsion, the Bose glass phase was predicted and studied theoretically and subsequently verified numerically.

Another reason for the increased interest in disordered bosonic systems is a set of fascinating experiments on atomic Bose-Einstein condensates on optical lattices. In many cases, such as this one, the relevant bosonic Hubbard model is the soft core one in others it is the hard core that is of interest. It is therefore interesting and important to expose and understand some of the important differences between these two cases.

The paper is organized as follows. In Sec. II we will first present the hard core boson Hubbard model, our simulation algorithm and measurements. Then, in Sec. III we will first review the phase diagram of the clean model before presenting our results on the disordered model at strong and weak near neighbor repulsions. Conclusions and comments are in section IV.

II. THE BOSON HUBBARD MODEL

The hard core boson Hubbard Hamiltonian is given by

\[ H = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \sum_i \mu_i n_i \]

\[ + V_1 \sum_{\langle ij \rangle} n_i n_j \]  \( \text{(1)} \)

\( a_i \) \( (a_i^\dagger) \) are destruction (creation) operators of hard–core bosons on site \( i \) of a two dimensional square lattice, and \( n_i \) is the boson number at site \( i \) while \( \mu_i \) is the site dependent chemical potential. This is, therefore, a site dependent energy which models the disorder in the system. In the absence of disorder, \( \mu_i \) becomes the normal chemical potential, \( \mu \). There are other ways to model disorder.
For example, one can have bond dependent hopping parameter \((t_{i,j})\), or near-neighbor interaction \((V_{1,i,j})\). It is thought, though not fully demonstrated, that these possibilities fall in the same universality class. The hopping parameter is chosen to be \(t = 1\) to fix the energy scale. \(V\) is the near neighbor interaction.

To characterize the different phases, we need to measure several physical quantities. A superfluid phase is characterized by the absence of long range density order and a non-vanishing superfluid (SF) density. The SF density, \(\rho_s\) is given by

\[
\rho_s = \langle W^2 \rangle/2t\beta, 
\]

where \(W\) is the winding number of the phase of the boson wave function in one of the two spatial dimensions and \(\beta = 1/kT\). Long range density order (such as in the checkerboard solid) is characterized by the density-density correlation function, \(c(l)\), and the structure factor, \(S(q)\), its Fourier transform. They are given by

\[
c(l) = \langle n_{j+i}n_j \rangle \\
S(q) = \sum_1 e^{iql} c(l), 
\]

where \(n_j\) is the occupancy at site \(j\). In the presence of long range order, \(S(q)\) will diverge with the system size for a given ordering momentum, \(q^*\), which characterizes the ordered phase. For example, for checkerboard order, \(q^* = (\pi, \pi)\).

Two other very useful quantities are the equal time Green’s function

\[
G(|j-i|) = \langle a_j a_i^\dagger \rangle, 
\]

and the Green’s function in imaginary time

\[
G(\tau) = \langle a_i \tau a_{i,0}^\dagger \rangle. 
\]

In the superfluid phase, \(G(|j-i|)\) saturates at a nonzero value for large separations, while \(G(\tau)\) tends to zero exponentially thus yielding the quasiparticle excitation energy spectrum. In the simulations, \(G(|j-i|)\) was measured along the lattice axes.

In the presence of disorder, we need to average over realizations of disorder in addition to the usual statistical average for a given realization. The number of realizations we used depended on the size of the system but is typically a few hundred. We do our simulations using the stochastic series expansion (SSE) algorithm with worm updates. This algorithm is numerically exact without any discretization error. In addition it uses non-local updates, hence even large systems can be sampled efficiently.

### III. THE PHASE DIAGRAM

The phase diagram of the bosonic Hubbard model with finite contact repulsion (i.e. soft core) and no nearest neighbor (nn) repulsion has been studied extensively in one and two dimensions both with and without disorder. In the absence of disorder, for incommensurate particle fillings, one always has a superfluid phase. This phase disappears at commensurate fillings (\(\rho = 1/2, 2/3\)) when the onsite repulsion is large enough. The resulting phase is an incompressible Mott insulating phase which takes the form of lobes in the \((t/V_0, \mu/V_0)\) plane, where \(V_0\) is the onsite repulsion. This phase is gapped, there is a substantial energy cost (increase in the chemical potential) for adding a particle onto a commensurate phase. It was argued that in the presence of any amount of disorder, a new compressible insulating (i.e. localized) phase, the bose glass, is produced at incommensurate fillings and that for strong enough disorder the gapped phase disappears entirely. This was subsequently confirmed numerically.

The picture changes for hard core bosons with near neighbor repulsion, \(V\). The bosons still form a superfluid for incommensurate particle filling and \(V\) not too strong. Also, at full filling, the bosons are always frozen into a Mott insulator since hopping to a neighbor would produce double occupancy which is strictly forbidden. At half filling, increasing \(V\) eventually freezes the bosons into an incompressible gapped checkerboard solid: Alternating sites are occupied since the presence of a neighbor costs too much energy and there is a big energy cost (gap) to add a particle. The phase diagram is shown in Fig. 1.

#### A. Strong Near Neighbor Repulsion

We now introduce disorder in the form of a random site dependent chemical potential, \(\mu_i = \mu + \delta_i\) where the disorder, \(\delta_i\) is uniformly distributed between \(\pm \Delta\). \(\Delta\) is a tunable parameter characterizing the strength of disorder. The first question we want to address is the strength of
the disorder necessary to destroy the checkerboard solid phase and what new phase is produced. One can try to answer this question with a simple argument based on energy balance (Imry-Ma). We start at half filling with a perfect checkerboard solid and introduce the site disorder. Suppose that at an empty site there is, due to \( \mu_i \), a deep potential well which pulls in a neighboring boson. This boson will now have near neighbors which it will try push away to rearrange its neighborhood in a local checkerboard solid which will, consequently, have a mismatch at its boundary with the original checkerboard. The likelihood of this happening depends on the disorder and dimensionality. The energy cost, in \( d \) dimensions, due to the mismatch at the boundary scales like \( L^{d-1} \) for a region of length \( L \). On the other hand, the energy gained by the bosons by falling into locally favorable energy wells scales like \( L^{d/2} \). For \( d = 1 \), disorder is relevant, no matter how weak it is, it always destroys the solid order. For \( d = 3 \) or more, the energy cost outweighs the gain and the system maintains checkerboard order. The \( d = 2 \) case is marginal since both, cost and gain, scale like \( L \). Typically, in such marginal cases, the conclusion is that disorder will indeed destroy long range order but just barely. The correlation length, \( \xi \), is very long and the system size should be even larger to see the effect.

Numerically, for strong disorder (\( \Delta/V = 2 \)) we can easily see that indeed the gapped checkerboard solid is destroyed on lattices as small as \( L = 12 \) and is replaced by a compressible, glassy insulator with no energy gap.

Since for very weak disorder, the system size needed to see the destruction of solid order is too large for us to simulate, we resort to finite size scaling for the intermediate disorder case. Although this does not demonstrate directly the validity of the Imry-Ma argument (for which very weak disorder is needed) we believe that the results we will present are qualitatively similar to what happens in the very weak disorder case.

In Figure 2 we show the density, \( \rho \), as a function of the chemical potential, \( \mu = \langle \mu_i \rangle \), for \( L = 8, 12, 14 \) (\( \beta = 14 \)) and \( L = 20 \) (\( \beta = 20 \)) and \( \Delta/V = 1 \). For \( L = 12, 14 \) and 20, we average 100 disorder realizations, for \( L = 8 \) we did 400. We see that the incompressible gapped region (\( \kappa = \partial \rho / \partial \mu = 0 \)) gets smaller as \( L \) increases but does not quite reach zero. The inset shows the average gap size versus \( L^{-1} \). The average gap size was obtained by calculating the \( \rho, \mu \) curve for each realization, which yields the gap size per realization which we then average. An alternative method (which washes out important statistical information) is to calculate the average \( \rho, \mu \) curve and use it to calculate the average gap. We see clearly that the gap tends to zero for a finite, but large, \( L \). This suggests that, for these values of \( V \) and \( \Delta \), the gap will disappear by \( L \approx 30 \). Since \( \rho \) should be greater than \( \xi \) to observe the destruction of the checkerboard order, we estimate from this that \( \xi \approx 30 \). In Figure 3 we show \( S(\pi, \pi) \) as a function of \( L^{-1} \). This, again, shows that the checkerboard order is destroyed for systems larger than about \( L = 30 \).

To elaborate this further, we show in Fig. 3 the distributions of the gap sizes for different disorder realizations for \( L = 8, 20 \). We see that for \( L = 8 \), the distribution is quite narrow and peaked at a nonzero value. However, for \( L = 20 \), the distribution is very wide and in fact peaked at zero indicating that the most probable value for the gap is zero. In this case, it is incomplete to discuss the “average” of the gap, which is still non-zero.

In order to characterize further the compressible phase which replaces the checkerboard solid, we study the behavior of the Green’s function, both for equal and unequal imaginary times. For example, in Figure 4 we show the equal time Green’s function for \( V = 4.5 \), \( L = 10 \) and \( \rho \approx 0.56 \). We see that the Green’s function goes to zero and is very well fit by an exponential (in fact a hyperbolic cosine to account for the periodic boundary conditions). This is further evidence that there is no superfluid in this phase, it is an insulator.
which has been verified numerically in a very different finite size scaling clearly shows the gap to disappear on finite lattice that the gapped solid phase is still present, results demonstrate that, whereas it might appear on a length will be even longer and much larger sizes would be needed. However, for moderate disorder, the above results demonstrate that, whereas it might appear on a finite lattice that the gapped solid phase is still present, finite size scaling clearly shows the gap to disappear on large enough systems. We may conclude from this that the Imry-Ma argument holds and that disorder, no matter how weak, will produce a glassy, compressible, ungapped insulating phase at strong near neighbor couplings.

B. Weak Near Neighbor Repulsion

We now consider the question of what happens when the near neighbor repulsion is decreased and only the hard core and disorder interactions remain. For soft core bosons with no nn interaction, a re-entrant behavior was observed for \( \rho_s \) as a function of the contact repulsion both in one and two dimensions. In other words, for fixed disorder strength, as the onsite repulsion is increased from zero, the superfluid density is at first zero, then at some intermediate value of \( V_0/t \) the bosons delocalize and \( \rho_s \) takes on a finite value, then for large enough \( V_0/t \) (i.e. approaching the hard core limit) the bosons are localized again. In one dimension this happens for any amount of disorder, but in two dimensions was only reported at \( \Delta/t = 6 \). This was taken as confirmation of the phase diagram presented in reference where the bosons were argued to be always localized, even by weak disorder, when \( V_0/t \) is very large.

The phase diagram in the \((t/V_0, \mu/V_0)\) plane should however be interpreted with care especially if we want to consider the hard core limit. It is a phase diagram at constant \textit{finite} disorder \( \Delta/V_0 \) and thus \( t/V_0 \to 0 \) means that \( \Delta/t \to \infty \), and any arbitrarily weak disorder in units of \( V_0 \) becomes infinitely strong in the hard core limit.

In fact, figure shows that hard core bosons behave differently, when a finite disorder \( \Delta/t \) is considered. While the bosons are localized by weak disorder for large nn coupling, \( V_1 \) (and densities that are not very small), as
this coupling is reduced, the bosons become superfluid and stay that way even at $V_1 = 0$. We verified this at several particle densities. In other words, the naive expectation based on the soft core phase diagram as presented in reference 2 at very large onsite repulsion is not fulfilled. The soft core phase diagram must be interpreted appropriately.

As we saw for the gap, in the presence of disorder it is not enough to consider only average quantities, it is also instructive to consider their distribution. In Figure 8 we show the histogram of $\rho_s/\rho$ for the 250 realizations for $L = 16, V = 0, \Delta/t = 5, \beta = 24$ and $\rho \approx 0.1$. We see that for this size the distribution is well centered around $\rho_s/\rho \approx 0.18$, with the same behavior observed for smaller sizes: The distribution does not widen nor does the peak tend to zero. Therefore, even for this large disorder, the bosons are still not localized for $V = 0$.

To show that the bosons can be localized at $V = 0$ if the disorder exceeds a threshold value, we show in Fig. 9 finite size scaling for $\rho_s/\rho$ for two cases of disorder, $\Delta = 5t$, and 6$t$. The case of $\Delta = 5t$ was done with $\rho = 0.1$ and clearly shows the system to be superfluid as as $L \to \infty$. This is also shown in the equal time Green’s function, Fig. 10. On the other hand for $\Delta = 6t$ we did the simulation at $\rho \approx 0.73$ and we find that both $\rho_s/\rho$ and the Green’s function vanish as $L \to \infty$. We also verified this for $\rho \approx 0.5$ and 0.1. We conclude that the disorder has to exceed a threshold value ($\approx 6t$) in order to localize the bosons for weak nn repulsion. Clearly, in the no-hopping limit, $t \to 0$, the critical value of the disorder vanishes in agreement with reference 2.

When the disorder is strong enough to localize the bosons at weak coupling and consequently also at strong coupling (since even very weak disorder can accomplish that), the question arises as to whether there is re-entrant behavior, as observed for soft core bosons. In other

FIG. 7: The Green’s function versus $r$ for $V = 0, \Delta = 5, \beta = 24, \rho = 0.1$ and $L = 8, 10, 12, 16$ showing that the system is superfluid. The inset shows $\rho_s/\rho$ versus $V$ for a 12X12 system. $\Delta/t = 5, \beta = 24, \rho = 0.1$ and 250 realizations. $\rho_s/\rho$ vanishes only for large $V$. The particle density is $\rho \approx 0.1$.

FIG. 8: Histogram of $\rho_s/\rho$ for the 250 realizations for $L = 16, V = 0, \Delta/t = 5, \beta = 24$ and $\rho \approx 0.1$.

FIG. 9: Finite size scaling of the superfluid density fraction $\rho_s/\rho$ for the pure hard-core case $V = 0$ for two different disorder strengths $\Delta = 5t$ and $\Delta = 6t$, $\beta = 20$.

FIG. 10: Finite size scaling of the equal time Green’s function at the largest distance for two different disorder strengths $\Delta = 5t$ and $\Delta = 6t$, $\beta = 20$.
words, will the bosons go from being localized at weak coupling to being delocalized at intermediate values and then relocalize at strong coupling? A finite size scaling analysis shows that this is not the case: For the hard core system, when the disorder is large enough to localize the bosons at weak coupling, they will stay localized at all couplings.

This means that the \((\mu/V, t/V)\) phase diagram is as follows. For weak disorder the checkerboard solid is completely destroyed and replaced by a compressible insulating Bose glass phase. This is easy to understand by applying to the two-sublattice structure of the checkerboard solid a simple Imry-Ma argument. However, away from half filling, there is no such structure and the Imry-Ma argument no longer holds. So, with weak disorder, there will be a superfluid even for large \(V\) repulsion, when the density is far from \(0.5\). In addition, there is a superfluid for all fillings (except full filling) when the \(V\) repulsion is small. For strong disorder, the superfluid phase everywhere is destroyed and replaced by the compressible Bose glass phase.

**IV. CONCLUSIONS AND DISCUSSION**

We have used the SSE algorithm to simulate the disordered hard core bosonic Hubbard model in two dimensions to try to understand the interplay and competition between interaction and disorder.

Using finite size scaling, we found that the checkerboard solid present at strong \(V\) interactions for half filling is completely destroyed by any amount of disorder. This agrees with the simple Imry-Ma energy balance argument.

Surprisingly, finite size scaling showed that at very weak, even vanishing, \(V\) coupling, weak (even intermediate) disorder does not localize the hard core bosons. The disorder strength, \(\Delta/t\), must be at least of the order of \(6t\) before the bosons are localized. We found this somewhat surprising because soft core bosons were argued to be always localized, even by weak disorder, in the limit \(t/V_0 \rightarrow \infty\) which is often considered to be equivalent to the hard core case. The soft core phase diagram should be interpreted carefully, as discussed in section III B.

Numerically, the bosons were shown to be localized but only one value of the disorder was presented, \(\Delta/t = 6\), which is large. Our numerical results here agree with reference 1, but show no localization for weaker disorder.

Another interesting analogy to make is with fermions. In one dimension, weak disorder localizes both fermions and hard core bosons, which is not surprising in view of the fact that they are equivalent in this case. In two dimensions, however, this equivalency is lost, and the response to disorder is different. Fermions are (marginally) localized by weak disorder while hard core bosons are not.

Since the hard core bosonic Hubbard model is equivalent to the spin-\(\frac{1}{2}\) quantum Heisenberg model, the above results also hold for this model in the presence of a random external magnetic field.

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