How localized bosons manage to become superfluid

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Received 9 June 2011
Accepted 5 July 2011
Published 8 August 2011

Online at stacks.iop.org/JSTAT/2011/P08004
doi:10.1088/1742-5468/2011/08/P08004

Abstract. We show that the many-body wavefunction built as a permanent of localized non-orthogonal single-particle states can describe bosonic superfluidity. The criterion for the transition is expressed in terms of the properties of the matrix of the overlaps between the single-particle wavefunctions. We apply this result to study the superfluid-to-Bose glass transition in a disordered Bose-Hubbard model through a very simple variational wavefunction. We finally consider a further quantity, the bipartite entanglement entropy, which also provides a good estimator for the superfluid-to-Bose glass transition.

Keywords: disordered systems (theory), Hubbard model (theory), optical lattices, superfluidity
1. Introduction

The study of the interplay between disorder and interaction has recently received novel impulse from the experimental realizations of correlated and disordered systems through optical lattices [1, 2]. Particular attention has been devoted to trapped bosonic atoms in the presence of on-site disorder, which can be simulated experimentally using speckles or superimposing incommensurate laser beams [3]–[5]. The great opportunity offered by such experiments is that not only can disorder be easily tuned but also can the interaction among the atoms, this latter by means of the Feshbach’s resonance technique [6]. These experiments have motivated a renewed theoretical activity on the phase diagram of the disordered Bose–Hubbard model [7]–[15], an old [16]–[21] but still debated issue. This model is supposed to exhibit three different phases. Besides the Mott insulating phase, occurring when interaction is strong and the particle density is commensurate, and the superfluid phase, stable for weak interaction, in the presence of disorder an additional phase has been predicted to occur [18], the so-called Bose glass. Such a disorder driven phase is supposed to be insulating but, unlike the Mott insulator, compressible. In the absence of interaction, the Bose glass is simply the state obtained by condensing all bosons in the lowest energy eigenstate of the single-particle disordered Schrödinger equation, which is supposed to lie in the Lifshitz tail of localized wavefunctions. This picture is, however, unstable to whatever weak interaction there is, since a macroscopic occupancy of a finite region in real space would be energetically impossible. In fact, a more realistic view of a Bose glass is that of disconnected superfluid droplets, where coherent inter-droplet tunneling is inhibited by the Anderson localization phenomenon—hence the insulating
How localized bosons manage to become superfluid behavior—but transferring electrons between different droplets is costless—hence the finite compressibility.

In this paper, we investigate the superfluid-to-Bose glass transition by means of a very simple variational wavefunction. It consists of a permanent of non-orthogonal single-particle wavefunctions that are determined in a variational manner. Although the approach is not as rigorous as e.g. a quantum Monte Carlo one \cite{8,10,13,15}, it nevertheless provides a very transparent description of the transition and of the same Bose glass. Indeed, all coherence properties of the wavefunction are hidden in the single-particle wavefunctions that build the permanent. In particular, since these wavefunctions need not be orthogonal, it is their overlap matrix that seems to play an important role. Actually one can derive an approximate criterion for the permanent to have macroscopic condensation at zero momentum, and hence superfluidity, which involves just the overlap matrix. We find that this criterion agrees well with the more rigorous one based on the superfluid stiffness.

Finally, in the last part of the paper we study the single-site von Neumann entropy, which could also be used to identify the superfluid-to-Bose glass transition. The quantum entanglement applied to many-body systems has attracted a lot of theoretical interest in recent years (see for instance \cite{22}–\cite{25} and references therein). So far, however, the entanglement witnesses have never been used in the context of a disordered Hubbard model. We show that, within our variational approach, the Bose glass seems to be characterized by a finite probability for the single-site von Neumann entropy to have zero value. In other words, as disorder increases, the entropy distribution gets broader and broader until the probability of having zero entropy becomes finite, which we identify as the onset of ‘Bose glassiness’. This criterion holds good qualitatively as long as we deal with small system size, since the zero entropy is the signature of vanishing charge fluctuations in some regions of the sample, which becomes then easily disconnected. A more quantitative analysis for large systems would involve the study of the entropy distribution and the appearance of the bimodal profile in agreement with the droplet scenario. Our conjecture is that the weights and the positions of the two modes at the transition should be related to the percolation threshold.

The paper is organized as follows. In section 2 we present a criterion for the onset of superfluidity that is based on the matrix of the overlaps between the single-particle wavefunctions that are used to build the variational many-body wavefunction. In section 3 we introduce the disordered Bose–Hubbard model and in section 4 we describe the variational many-body wavefunction that we study. Section 5 is devoted to studying the bipartite entanglement entropy as another tool for identifying the superfluid-to-Bose glass transition. Final conclusions are summarized in section 6.

2. The overlap matrix criterion

Let us imagine a Hartree–Fock-like variational approach to the problem of disordered and interacting bosons that amounts to searching for the permanent that minimizes the total energy. Unlike conventional Hartree–Fock theory for fermions, such an approximation for bosons does not lead to significant simplifications with respect to exact numerical simulations because permanents are extremely difficult to handle. Nonetheless, let us assume that we have successfully performed the calculation and found the optimal
permanent for \( N \) particles, which can be written as

\[
|\Psi\rangle = \prod_{\alpha=1}^{N} \left( \sum_i \psi_{\alpha i} b_i^\dagger \right) |0\rangle,
\]

in terms of a set of single-particle wavefunctions \( \psi_\alpha \), with amplitude \( \psi_{\alpha i} \) at site \( i \). In (1) \( b_i^\dagger \) creates a boson at site \( i \). Unlike Slater determinants, the wavefunctions that built a permanent need not be orthogonal to one another, so we expect the overlap matrix \( \Omega \) to have non-zero off-diagonal elements \( \Omega_{\alpha\beta} = \sum_i \psi_{\alpha i} \psi_{\beta i}^* \). For instance, if all bosons condense into a single state, then all \( \psi_\alpha \) are equal and \( \Omega_{\alpha\beta} = 1, \forall \alpha, \beta \in [1, N] \). In the generic case where the \( \psi_\alpha \) are distinct, we may wonder whether wavefunction (1) describes a superfluid. In what follows we derive a simple criterion that is based on the properties of the overlap matrix.

One can verify that the norm of (1) can be written as an integral over classical variables as [18]

\[
\langle \Psi | \Psi \rangle = \int \prod_{\alpha} \frac{d\xi_\alpha}{\pi} d\xi_\alpha^* e^{-S(\xi, \xi^\dagger)}
\]

with the following action (see appendix A):

\[
S(\xi, \xi^\dagger) = \xi^\dagger (\Omega - I)^{-1} \xi - \sum_\alpha \ln(1 + |\xi_\alpha|^2).
\]

We assume that the main contribution to the integral comes from the saddle point, i.e. the solution of

\[
\xi_\alpha = \sum_\beta (\Omega_{\alpha\beta} - \delta_{\alpha\beta}) \frac{1}{1 + |\xi_\beta|^2} \xi_\beta.
\]

The above equation implies that finite values of \( \xi_\alpha \) appear in groups, or equivalently that \( \Omega \) is a block matrix. In the presence of disorder this is suggestive of the existence of clusters occupied by bosons whose wavefunctions mutually overlap. Because of interaction, a cluster cannot accommodate all particles unless it covers all of the system, which would correspond also to superfluidity. If we linearize (4), we find that the condition for the appearance of a cluster reads

\[
\xi_\alpha = \sum_\beta (\Omega_{\alpha\beta} - \delta_{\alpha\beta}) \xi_\beta,
\]

which corresponds to a block of \( \Omega \) that acquires an eigenvalue greater than 2. As we mentioned, this is still not the condition for superfluidity. The latter rather implies that a block in \( \Omega \) should grow, or several blocks should merge, i.e. start to overlap, until a percolating cluster emerges. This condition is likely to be equivalent to an eigenvalue of \( \Omega \) growing with the number of bosons \( N \). We finally mention that the saddle point approximation that we used is rigorously valid only if blocks are big enough.
2.1. The density matrix and the overlap condition

A better and more transparent criterion for detecting a long-range order is obtained by resorting to the definition of the density matrix:

$$C_{ij} = \langle \Psi | b_i^\dagger b_j | \Psi \rangle. \quad (6)$$

Off-diagonal long-range order implies that $C_{ij}$ is finite for $|i - j| \to \infty$. Within the path integral formulation, using equations (A.2), (A.6), one can verify that $C_{ij}$ can be written as

$$C_{ij} = \sum_{\alpha\beta} \psi_{i\alpha}^\dagger \langle \xi_{\alpha} \xi_{\beta}^\dagger \rangle \psi_{\beta j}. \quad (7)$$

where $\langle \cdots \rangle$ is now the average weighted by $e^{-S}$, with the action $S$ given by equation (3). If the saddle point of the action is characterized by finite $\xi_{\alpha}$, one could be tempted to set

$$\langle \xi_{\alpha} \xi_{\beta}^\dagger \rangle \simeq \langle \xi_{\alpha} \rangle \langle \xi_{\beta}^\dagger \rangle. \quad (8)$$

This is not fully correct. Indeed, if $\Omega$ is a block matrix, within each block only the relative phases of the $\xi_{\alpha}$ are fixed, while an overall phase is still free and has to be integrated out. This implies that (8) is correct only if $\alpha$ and $\beta$ are within the same block; otherwise the relative phase of the two blocks will suppress the average. This suggests that off-diagonal long-range order sets in only if a single block percolates. More rigorously, we define

$$\xi_i = \sum_{\alpha} \psi_{i\alpha}^\dagger \xi_{\alpha}, \quad (9)$$

through which the density matrix reads

$$C_{ij} = \langle \xi_i \xi_j^\dagger \rangle. \quad (10)$$

The saddle point equation in terms of $\xi_i$ is

$$2 \xi_i = \sum_j O_{ij} \xi_j, \quad (11)$$

where

$$O_{ij} = \sum_{\alpha} \psi_{\alpha i}^* \psi_{\alpha j}, \quad (12)$$

is the density matrix of the wavefunctions. An extreme superfluid solution identified by $\xi_i = \xi, \ \forall i$, could be stabilized if

$$\mathcal{F} \equiv \frac{1}{N_s} \sum_{ij} O_{ij} \geq 2, \quad (13)$$

where $N_s$ is the number of sites.

doi:10.1088/1742-5468/2011/08/P08004
2.2. An example: the bosonic crystal

As a simple application of the previous results we shall now investigate the possibility that a permanent that describes at the ‘Hartree–Fock’ level a Bose–Wigner crystal, could also be superfluid, actually a supersolid. Let us consider a commensurate density $N/N_s < 1$ of interacting bosons on a lattice with $N_s$ sites in the absence of disorder. If the repulsion is sufficiently strong and long-ranged, we may imagine that the best variational permanent wavefunction describes a bosonic superlattice with Bravais vectors

$$\mathbf{R} = a(m_1, m_2, \ldots, m_d),$$

where $a$ is the superlattice parameter. We write the Wannier single-particle wavefunctions that correspond to the Bose–Wigner crystal as

$$\psi_{\mathbf{R}}(\mathbf{R}_i) = \sqrt{\frac{1}{N_s}} \sum_{\mathbf{k}} u_{\mathbf{k}} e^{i \mathbf{k} (\mathbf{R} - \mathbf{R}_i)},$$

where $\mathbf{k}$ runs within the Brillouin zone of the original lattice, and $\mathbf{R}_i$ spans all lattice sites, while $\mathbf{R}$ spans only the superlattice ones. The permanent is therefore

$$|\Psi\rangle = \prod_{\mathbf{R}} \left( \sum_{\mathbf{R}_i} \psi_{\mathbf{R}}(\mathbf{R}_i) \right) |0\rangle.$$  

In this case the overlap matrix is

$$\Omega_{\mathbf{R} \mathbf{R}'} = \frac{1}{N_s} \sum_{\mathbf{k}} |u_{\mathbf{k}}|^2 e^{i \mathbf{k} (\mathbf{R} - \mathbf{R}')}.$$  

We assume for simplicity that the wavefunction is Gaussian:

$$u_{\mathbf{k}} = \frac{1}{v} \left( \frac{\ell}{\sqrt{\pi}} \right)^d e^{-\ell^2 |\mathbf{k}|^2 / 4\pi^2},$$

where $v$ is the volume of unit cell and $\ell$ the localization length, so the overlap matrix has the simple expression

$$\Omega_{\mathbf{R} \mathbf{R}'} = e^{-\pi^2 (|\mathbf{R} - \mathbf{R}'|^2 / \ell^2)},$$

and depends only on the distance, $\Omega_{\mathbf{R} \mathbf{R}'} = \Omega_{\mathbf{R} - \mathbf{R}'}$. From the saddle point equation we find that the condition for having superfluidity is simply

$$\sum_{\mathbf{R}} \Omega_{\mathbf{R}} = \sum_{\mathbf{R}} e^{-\pi^2 (|\mathbf{R}|^2 / \ell^2)} \geq 2.$$  

By means of the Jacobi theta function $\theta_3(0|x) = \sum_{m=-\infty}^{\infty} x^{2m}$, equation (20) means

$$\theta_3(0|e^{-\pi^2 a^2 / \ell^2}) \geq \sqrt{2}.$$  

The condition of equation (21) fixes the critical overlap between the Wannier functions, parameterized by the ratio $\ell/a$, above which bosons condense at zero momentum, i.e. the many-body wavefunction describes a supersolid.

In section 3 we shall consider the Bose–Hubbard model in the presence of disorder which causes now the localization of the single-particle wavefunctions. We are going to see that, also in that case, in spite of the Anderson localized nature of the single-particle states obtained variationally, the many-body wavefunction can be a superfluid one.
3. The model

We consider a system of interacting bosons on a disordered two-dimensional lattice with \( N_s = L^2 \) sites, described by the following Bose–Hubbard Hamiltonian:

\[
H = -\frac{t}{2} \sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{H.C.}) + \sum_i \epsilon_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1),
\]

(22)

where \( b_i^\dagger \) (\( b_i \)) creates (annihilates) a boson at site \( \mathbf{R}_i \), \( \langle ij \rangle \) denotes the sum over all pairs of neighboring sites, \( n_i = b_i^\dagger b_i \) is the boson local density, and, finally, the \( \epsilon_i \) are random on-site energies uniformly distributed between \( -\Delta \) and \( \Delta \).

Since the seminal works of Giamarchi and Schulz [16, 17] and Fisher et al [18], the Hamiltonian (22) has been studied with a variety of techniques, mainly in one and two dimensions. More recently, highly sophisticated numerical simulations [7, 8, 10], [13]–[15], [20, 21] have been performed to uncover the full phase diagram and settle some debated issues, like the possibility of a direct superfluid Mott insulator transition. The results that we are going to present are by no means comparable in accuracy with the aforementioned numerical simulations. Our main purpose is not to compete with those simulations, but just to provide an interpretation of the phase diagram in terms of a simple Hartree–Fock-like single-particle picture.

4. The method

The simplest way to deal with interacting electrons is by using the Hartree–Fock approximation, which amounts to searching for the best wavefunction within the subspace of Slater determinants. This approximation reduces the complicated many-body problem to a single-particle one with an effective potential generated by all other particles. Even more realistic approaches, like that of the density functional theory in the local density approximation, eventually reduce to the self-consistent solution of a single-particle Schrödinger equation. The great advantage is that a single-particle description is very intuitive and, although it could be too naive in many cases, at least it is a simple starting point for more complicated approaches.

The obvious generalization of the Hartree–Fock approximation to interacting bosons would involve searching for the best wavefunction within the subspace of permanents, the bosonic analogs of Slater determinants. However, as we already mentioned, unlike Slater determinants, permanents are well defined even if the single-particle wavefunctions that are used are not orthogonal to each other. Therefore the optimization procedure is not reduced to solving a single eigenvalue problem, which would produce a set of orthogonal wavefunctions, but becomes rather complicated, and practically unfeasible, and hence further approximations are required [26].

Our simplified approach consists in adding one boson at a time, with a wavefunction that is the ground state of a non-interacting Hamiltonian with a potential determined by the already added bosons. Specifically, we consider the non-normalized \( N \)-boson wavefunction

\[
|\Psi_N \rangle = \prod_{\alpha=1}^N \left( \sum_j \chi_{\alpha j} b_j^\dagger \right) |0\rangle
\]

(23)
where the $\chi_{\alpha j}$, $j = 1, \ldots, N_s$, are generically non-orthogonal single-particle wavefunctions. The first wavefunction $\chi_{1j}$ is the ground state of (22) with $U = 0$ (no bosons are present). The $(M + 1)$th wavefunction is instead the ground state of

$$H_{\text{app}} = -\frac{t}{2} \sum_{ij} b_i^\dagger b_j + \sum_i (\epsilon_i + U \langle n_i \rangle) n_i,$$

where

$$\langle n_i \rangle = \frac{\langle \Psi_M | b_i^\dagger b_i | \Psi_M \rangle}{\langle \Psi_M | \Psi_M \rangle}$$

is the average density of the previously added $M$ bosons. We define an $M \times M$ matrix

$$\Omega_{\alpha\beta} = \sum_{i=1}^{N_s} \chi_{\alpha i} \chi_{\beta i}^*$$

with $\alpha, \beta = 1, \ldots, M$, and, for each couple of lattice sites $(i, j)$, the $(M + 1) \times (M + 1)$ matrices

$$D_{ij} = \begin{pmatrix} \Omega_i & \hat{\chi}_i \\ \hat{\chi}_j^t & \delta_{ij} \end{pmatrix}$$

where $\hat{\chi}_i = (\chi_{1i}, \ldots, \chi_{Mi})^t$. It follows that the mean local density that is required for adding the next $(M + 1)$th boson, namely equation (25), can be written as follows:

$$\langle n_i \rangle = \frac{\text{Per}(D_{ii})}{\text{Per}(\Omega)} - 1$$

where $\text{Per}(X)$ is the permanent of $X$. At each iteration, one can also calculate the intersite density matrix, since

$$C_{ij} \equiv \frac{\langle \Psi | b_i^\dagger b_j | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\text{Per}(D_{ji})}{\text{Per}(\Omega)} - \delta_{ij},$$

and hence investigate the eventual offset of long-range order. This procedure is iterated until the desired number $N$ of bosons is reached. We note that the method can be easily extended to study excited states—it is sufficient to select at any iteration not the ground state but an excited one—and hence at finite temperature, even though in what follows we just focus on the lowest energy states.

The superfluid properties of the model can be accessed by calculating the superfluid stiffness $\rho_{sf}$ defined through

$$\rho_{sf} \simeq \frac{L^2}{N} \frac{\partial^2 E_\theta}{\partial \theta^2} |_{\theta = 0},$$

where $E_\theta$ is the average value of the Hamiltonian (22) with twisted boundary conditions along a given direction $\mathbf{x}$, or, alternatively, with the parameter for hopping between neighboring sites $t_{ij} = t e^{i \theta \hat{r} \cdot \hat{x}}$, where $\hat{r} = (\mathbf{R}_i - \mathbf{R}_j)/L$. In terms of permanents we calculate

$$E_\theta = -\sum_{ij} \left( \frac{t_{ij}}{2} - \delta_{ij} (\epsilon_i - 2U) \right) C_{ij} + \frac{U}{2} \sum_i \left( \frac{\text{Per}(I_{iii})}{\text{Per}(\Omega)} - 2 \right)$$

where

$$I_{ij} = \begin{pmatrix} \Omega_i & \hat{\chi}_i \\ \hat{\chi}_j^t & \delta_{ij} \end{pmatrix}$$

and

$$I_{ij} = \begin{pmatrix} \Omega_i & \hat{\chi}_i \\ \hat{\chi}_j^t & \delta_{ij} \end{pmatrix}$$

doi:10.1088/1742-5468/2011/08/P08004
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**Figure 1.** Contour plot of the superfluid stiffness $\rho_{sf}$, equation (29), for a $6 \times 6$ square lattice at filling $\nu = 1/4$, averaging over 400 disorder configurations. The two thick dashed lines and the dotted line show the border of the superfluid phase, obtained by looking at some indicators related to the overlap matrix, as discussed in section 4.1.

where $C_{ij}$ is defined in equation (28) and $\text{Per}(I_{ijkl}) = \langle \Psi | b_i b_j ^\dagger b_k ^\dagger b_l ^\dagger | \Psi \rangle$ with

$$I_{ijkl} = \begin{pmatrix} \Omega & \tilde{x}_i & \tilde{x}_j \\ \tilde{x}_k ^\dagger & \delta_{ik} & \delta_{jk} \\ \tilde{x}_l ^\dagger & \delta_{il} & \delta_{jl} \end{pmatrix}. \quad (31)$$

Upon repeating this calculation for several disorder configurations, averaging over them and setting equal to zero the stiffness in the region of parameters where its variance is greater than its average (cutting off, therefore, the values of $\rho_{sf}$ that are statistically undetermined), we finally obtain the phase diagram of figure 1, which is a contour plot of the averaged superfluid stiffness $\rho_{sf}$ of a two-dimensional model with filling fraction $\nu = N/N_s = 1/4$. We note that in a finite system there cannot be a true gauge symmetry breaking; hence the phase diagram figure 1 is just an indication of what could happen in the thermodynamic limit. Nevertheless, the qualitative behavior that we find is physically sensible: $\rho_{sf}$ decreases with increasing disorder and, at fixed disorder, first increases with $U$ and then diminishes. In figure 1 and in the following figures the values of $U$ and $\Delta$ are in units of $t$.

We previously mentioned that a realistic view of a Bose glass is that of disconnected droplets. A way to confirm this idea is by plotting the average density as shown in figure 2, where we used, instead of equation (25), $\langle n_i \rangle \simeq \sum_{i} |\chi_{ai}|^2$, which is a good approximation for local densities, in order to computationally reach larger system sizes. We find that, at large disorder, bosons are indeed concentrated into droplets whose magnitude increases.

doi:10.1088/1742-5468/2011/08/P08004
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Figure 2. Contour plot of the particle density $\langle n_i \rangle$ on a $28 \times 28$ lattice with $N = 49$ bosons, i.e. filling $\nu = 1/16$, at $U = 10$ and for a single realization of disorder with $\Delta = 1, 2, 3$ from right to left (i.e. crossing the transition; see the inset of figure 6). The darker the sites, the higher the density.

with decreasing disorder until a percolating cluster appears, which must presumably signal the onset of the superfluid.

4.1. Comparison with the overlap matrix method

Let us compare the transition obtained from the superfluid stiffness with that given by the overlap matrix criterion. In our case, given the many-body wavefunction of equation (23), the overlap matrix $\Omega$ is that defined in equation (26) with $\psi_{\alpha i} = \chi_{\alpha i}$. The action is given by equation (3) and the saddle point equation reads as in equation (5), which has nontrivial solution if $\Omega$ has eigenvalue 2.

In figure 1 we plot a dotted line below which $(\Omega - 2I)$, or equivalently, $(\mathcal{O} - 2I)$, has both positive and negative eigenvalues for any disorder configuration, implying that the saddle point equation always has nontrivial solutions. Above that line, instead, for some disorder configurations all the eigenvalues of $\Omega$ are smaller than 2.

In the same figure, figure 1, we plot two thick dashed lines which correspond to $\bar{F} = 2$ (the upper line), namely, when the value of $\mathcal{F}$ as defined in equation (13), averaged over 400 disorder configurations, equals 2, and $\min(\mathcal{F}) = 2$ (lower line), namely, when the minimum value of $\mathcal{F}$ among the disorder configurations equals 2. Below those lines the corresponding quantities exceed the threshold value. Notice that a nontrivial solution of the saddle point equation occurs also for large disorder and weak interaction (the dotted line keeps on growing with decreasing $U$) while $\mathcal{F}$, which detects the long-range order (dashed lines), follows correctly the stiffness behavior also for small interaction.

In summary, we find that the superfluid properties of the many-body wavefunction (23) can be related to the matrix $\Omega$ of the overlaps between the single-particle wavefunctions $\chi_{\alpha i}$. This result also clarifies why, even though each wavefunction $\chi_{\alpha i}$ is the lowest energy solution of the Schrödinger equation of a particle in a disordered potential, and hence would always be localized in two dimensions, and also in higher dimensions if, as presumably is the case, it lies in the Lifshitz tail, nevertheless the permanent built with them could still be superfluid.

A final comment. We optimized the wavefunction by explicitly evaluating permanents. This is in general very onerous, not much simpler than an exact numerical solution of the problem, which is why our simulation size is small. However, we could adopt
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Figure 3. Eigenvalues of $\Omega$ as functions of $\Delta$, at a given configuration of disorder, for 49 bosons on a square lattice with 256 sites, namely always for filling $1/4$, at $U = 10$. The inset magnifies the lower part of the main plot.

an oversimplified approach and evaluate the Hartree potential in equation (24) for the $(M + 1)$th boson using

$$\langle n_i \rangle \simeq \sum_{\alpha=1}^{M} |\chi_{\alpha i}|^2,$$

as if the already present $M$ bosons were distinguishable. This approximation simplifies a lot the procedure for determining the single-particle wavefunctions, which can be pushed to very large system sizes. These single-particle wavefunctions can then be used to construct the permanent, whose superfluid properties can be assessed using the overlap matrix criterion. Even though such a procedure is hardly justifiable from the variational point of view, it provides a phase diagram that is qualitatively correct. Using this approximation, one can study the spectrum of the overlap matrix $\Omega$ for a larger system, finding that the transition is indeed characterized by the fact that the greatest eigenvalue of $\Omega$ starts growing toward the value $N$, the number of bosons, for $\Delta$ going to zero. From figure 3 one can see clearly, in fact, that a single eigenvalue of $\Omega$ (although quite noisy, it is a single level) separates from the others at $\Delta \approx 4$, approximately at the same value of disorder as was obtained for a smaller system size with $\langle n_i \rangle$ given by (27) (cf the transition line at $U = 10$ in figure 1). The other eigenvalues (see the inset of figure 3) accumulate around 0 below the transition, and around 1 above it, at least for filling not greater than 1, as in our case.

5. Spatial entanglement entropy

Another quantity which may be interesting to look at is the single-site entanglement entropy. We define as $\rho_n(i)$ the probability of having $n$ bosons at site $i$, which must trivially satisfy $\sum_{n=0}^{N} \rho_n(i) = 1$, where $N$ is the total number of bosons. The single-site
entr tray $S_i$ is thus defined through

$$S_i = - \sum_{n=0}^{N} \rho_n(i) \ln \rho_n(i).$$

In a disordered system it is also convenient to define its probability distribution through

$$P(S) = \left\langle \frac{1}{N_s} \sum_i \delta(S - S_i) \right\rangle_{\text{disorder}},$$

which is obtained by considering all sites and all disorder configurations. We are going to show that, in spite of its simple definition, the single-site entanglement entropy and, especially, its distribution probability are quite enlightening quantities in the presence of both disorder and interaction.

5.1. A limiting case

We start by considering the case where all bosons condense into a single state, i.e. $\chi_{\alpha j} = \zeta_j$, $\forall \alpha$, with the normalization condition $\sum_{j=1}^{N_s} \zeta_j = 1$. In this case $\text{Per}(\Omega) = N!$ and the state equation (23), including the normalization factor $1/\sqrt{\text{Per}(\Omega)}$, can be decomposed in the site Fock basis as

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \left( \sum_j \zeta_j b_j^\dagger \right)^N |0\rangle = \sum_{\{n\}} \sqrt{N!} \prod_{i=1}^{N_s} \zeta_i^{n_i} (b_i^\dagger)^{n_i} |0\rangle.$$

This is a diagonal $(N+1)!/(\ell!(N+1-\ell)!) \times ((N+1)!/(\ell!(N+1-\ell)!))$ matrix. For each diagonal element $\rho_{n_1,\ldots,n_\ell}$, corresponding to the configuration of the occupation numbers $(n_1, n_2, \ldots, n_\ell)$ of the $\ell$ sites that are not traced out, we obtain the following expression:

$$\rho_{n_1,\ldots,n_\ell} = \frac{1}{(N - \sum_{i=1}^{\ell} n_i)! \prod_{i=1}^{\ell} n_i!} \left(1 - \frac{1}{N} \sum_{i=1}^{\ell} \zeta_i^2\right)^{N - \sum_{i=1}^{\ell} n_i} \prod_{i=1}^{\ell} |\zeta_i|^{2n_i}.$$

From now on we shall focus on the simplest partitioning, keeping only one site and tracing over all the others, i.e. $\ell = 1$. In this case we get a very simple binomial expression for the reduced density matrix $\rho_n \equiv \rho_n(1)$:

$$\rho_n = \binom{N}{n} \left(1 - |\zeta_1|^2\right)^{N-n} |\zeta_1|^{2n}.$$
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Figure 4. Single-site entanglement entropies obtained from equations (38), (33). Upper dotted line: the maximum entropy, reached when $|\zeta_1|^2 = 1/2$. Upper middle dotted line: the entropy for the superfluid for the $\nu = 7/2$ case, i.e. for $|\zeta_1|^2 = 7/(2N)$. Lower middle dotted line: the entropy for the superfluid in the commensurate $\nu = 1$ case, i.e. for $|\zeta_1|^2 = 1/N$. Lower dotted line: the superfluid entropy for $|\zeta_1|^2 = 1/(4N)$, i.e. $\nu = 1/4$.

It is straightforward to check that $\sum_n \rho_n = 1$. The reduced density matrix is fully local; it depends only on the value of the wavefunction $\zeta$ on that site. We can now calculate the entanglement von Neumann entropy at site 1, $S_1$, through (33). From equations (38) and (33) we find that for any fixed value of $|\zeta_1| \in (0, 1)$ and for large $N$, the asymptotic value of $S_1$ is

$$S_1 \xrightarrow{N \gg 1} S_{loc} \equiv \frac{1}{2} \ln N + A,$$

with $A = \frac{1}{2} \{ 1 + \ln[2\pi |\zeta_1|^2(1 - |\zeta_1|^2)] \}$. At the two extremes, $|\zeta_1| = 0, 1$, we have $S_1 = 0$.

Let us consider first the non-interacting case with disorder. All bosons condense into a localized wavefunction. Within the localization region, $S_i \sim \ln N$, while outside, $S_i = 0$. We conclude that the probability distribution (34) becomes peaked at the single value $S = 0$ in the thermodynamic limit, $N_s \to \infty$, where the localization region has zero measure with respect to the whole system.

In contrast, without disorder and deep in the superfluid phase, for small $U$, we expect that

$$|\zeta_1|^2 = \frac{1}{N_s} = \frac{\nu}{N},$$

where the filling fraction $\nu = N/N_s$. In this case, the single-site entropy in the thermodynamic limit is finite and site independent, and depends exclusively on the filling fraction $\nu:

$$S_1 \xrightarrow{N \to \infty} S_{SF} \equiv \nu (1 - \ln \nu) + e^{-\nu} \sum_{n=0}^\infty \frac{\nu^n}{n!} \ln n!. $$

The sum equation (41) converges for any value of $\nu$. As one can see from figure 4, the thermodynamic limit, equation (41), is approached already with few bosons, for small $\nu$. 

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Figure 5. Probability distribution of the entropy for \( U = 10 \) and for different values of the disorder strength (\( \Delta = 1, 2, 4, 6 \)). The plot has been produced after \( 10^4 \) realizations of disorder in a system of \( N = 4 \) bosons on a \( 4 \times 4 \) square lattice. In the inset: the fluctuations of \( S \) increase with the strength of the disorder and saturate to the maximum value of the entropy for four bosons, which is \( \approx 1.4 \).

In the same figure we also draw the maximum entropy line, equation (39), which does indeed lie above all curves.

In conclusion, we expect the probability distribution of the single-site entropy to be peaked at a finite value deep in the superfluid phase but at value zero deep in the Bose glass phase. The obvious question is that of what happens in between.

5.2. Single-site entropy across the superfluid-to-Bose glass transition

Let us now consider the state in equation (23), including the normalization factor \( 1/\sqrt{\text{Per}(\Omega)} \), which in the Fock basis of sites reads

\[
|\Psi\rangle = \frac{1}{\sqrt{\text{Per}(\Omega)}} \sum_{\{n\} \{\{p_j\}\}} n_j^{N_s} \prod_{j=1}^{N} \chi_{p_j(\alpha)j} (b_j^\dagger)^{n_j} |0\rangle. 
\] (42)

The sum runs over \( \{n\} = (n_1, n_2, \ldots, n_{N_s}) \), the configurations of occupation numbers with the constraint \( \sum_i n_i = N \), and over \( \{\{p_j\}\} \) with \( \sum_{\{\{p_j\}\}} = \sum_{\{p_1\}} \sum_{\{p_2\} \neq \{p_1\}} \sum_{\{p_3\} \neq \{p_1\}, \{p_2\}} \cdots \) where \( p_j(\alpha) \) is the particle label which takes \( n_j \) integer values among \( N \) values. The reduced density matrix for a single site is found to be

\[
\rho_n = \frac{n!}{\text{Per}(\Omega)} \sum_{n_2, \ldots, n_{N_s}} n_i! \left| \sum_{\{\{p_j\}\}} n_j^{N_s} \prod_{j=1}^{N} \chi_{p_j(\alpha)j} \right|^2. 
\] (43)

The explicit expressions for the reduced density matrix for \( N = 2 \) and \( 4 \) are given in appendix B. In what follows we will consider the simple case of \( N = 4 \) bosons. In figure 5 we show the probability distribution of the single-site entanglement entropy.
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Figure 6. The minimum site entanglement entropy $S_{\text{min}}$ (light green lines) compared with the superfluid stiffness $\rho_{sf}$ (dark red lines) as functions of the disorder, for $U = 10$ and for filling fraction $\nu = 1/4$ (main plot) and $\nu = 1/16$ (inset). The stiffness, $\rho_{sf}$, is taken as an average among 400 configurations of disorder for a system of $N = 9$ bosons on a square lattice of $6 \times 6$ ($\nu = 1/4$, main plot) and $12 \times 12$ ($\nu = 1/16$, inset). The minimum entropy $S_{\text{min}}$ is obtained taking the minimum values of $S$ among $10^4$ configurations of the disorder, and for $N = 4$ on a $4 \times 4$ ($\nu = 1/4$, main plot) and $8 \times 8$ ($\nu = 1/16$, inset) lattices. The blue arrows point at the transitions, obtained from the overlap matrix method as explained in section 2.

which, in the absence of disorder, is peaked around $S \approx 0.62$, broadens under the action of disorder and finally, when disorder becomes strong, again develops a peak but at $S = 0$. We observe that the probability of having zero entropy becomes non-zero only above a disorder threshold that occurs approximately when also the stiffness vanishes, as one can see from figure 6.

We have found that in our finite size simulation the crossover between the two limiting behaviors, $P(S)$ peaked either at $S \neq 0$, deep in the superfluid, or close to $S = 0$, deep in the Bose glass, is continuous. We have also noticed that the point at which $P(S)$ becomes finite at $S \approx 0$ seems to coincide with the point where the stiffness becomes very small, which could be taken as the finite size signal of the superfluid-to-Bose glass transition. This suggests that the behavior of $P(S = 0)$ could be used also to identify the superfluid-to-Bose glass transition as an alternative to the superfluid stiffness in any finite size numerical simulations. Moreover, we note, looking at figure 5, that, close to the transition ($\Delta \approx 4$), the profile of the distribution (the green curve) is an almost equally weighted bimodal, peaked both at small $S$ (insulating regions) and at $S = S_{\text{SF}}(\nu_{\text{eff}})$ (superfluid regions) given by equation (41) where $\nu$ is replaced by $\nu_{\text{eff}} = \nu/p_c$. The numerical result for the second peak close to the transition ($S \approx 0.8$, for $\nu = 1/4$) is consistent with $p_c \approx 0.59$ which is the site percolation threshold for a square lattice. We have checked this result also with other filling fractions. This finding is in nice agreement with the percolating droplets scenario.

doi:10.1088/1742-5468/2011/08/P08004
6. Conclusions

We have considered a two-dimensional Bose–Hubbard Hamiltonian in the presence of disorder, and constructed a trial many-body wavefunction by solving a single-particle problem for one boson at a time, that feels the effect of all the others as an effective potential. By means of this wavefunction we have studied the transition between the superfluid and the Bose glass. We find that the transition can be characterized by, besides the vanishing stiffness, the eigenvalues of the matrix of the overlaps between the single-particle wavefunctions. Another quantity that we propose to look at is the single-site entanglement entropy. In particular, we argue that when the probability of measuring zero entropy becomes finite, \( P(S = 0) > 0 \), the superfluid starts to vanish and the Bose glass phase sets in. The bimodal entropy distribution is, then, the signature of a lack of percolation among superfluid clusters.

Appendix A: Derivation of the action

Let us consider the following wavefunction:

\[
|\Psi\rangle = \prod_{\alpha} \left( \sum_i \psi_{\alpha i} b_i^\dagger \right)^{n_\alpha} |0\rangle,
\]

which generalizes equation (1) where the integers \( n_\alpha \) are all equal to 1. Let us define also the overlap matrix \( \Omega_{\alpha\beta} = \sum_i \psi_{\alpha i} \psi_{\beta i}^* \) which is Hermitian and positive definite, such that it can be parametrized as \( \Omega = \psi \psi^\dagger = V^\dagger |\lambda|^2 V \), in terms of a unitary matrix \( V \). Let us suppose now that another unitary matrix \( U \) exists such that we can write \( \psi = V^\dagger \lambda U \), and define the following bosonic operators:

\[
b_a^\dagger = \sum_i U_{ai} b_i^\dagger
\]

\[
b_a^\dagger = \sum_a V_{aa}^\dagger b_a^\dagger.
\]

Defining also

\[
e^T \equiv \sum_a b_a^\dagger b_a \ln \lambda_a
\]

one can then verify that

\[
\sum_i \psi_{\alpha i} b_i^\dagger = \sum_a V_{aa}^\dagger \lambda_a b_a^\dagger = e^T b_a^\dagger e^{-T}
\]

where we have used the Hausdorff relation

\[
\lambda_a b_a^\dagger = e^T b_a^\dagger e^{-T}.
\]

Therefore equation (A.1) can be written as follows:

\[
|\Psi\rangle = e^T \prod_{\alpha} \left( b_a^\dagger \right)^{n_\alpha} |0\rangle.
\]
Moreover, one can check that
\[ e^{T^\dagger T} = e^{\sum a \hat{b}_a^\dagger \hat{b}_a} \ln |\lambda_a|^2 = \frac{1}{\pi} \int \prod_a dz_a \, dz_a^* \, e^{-\sum a |z_a|^2} \, e^{\sum_a z_a^* \hat{b}_a^\dagger} \, e^{\sum_a z_a \hat{b}_a} \]  
(A.8)

with \(|\lambda_a|^2 = 1 + |a|^2\). Now, in order to rewrite equation (A.8) on the basis of \(b_a\), we have to define \(\hat{v}_{ai} = \sum_a V_{ai}^\dagger v_a U_{ai}\) and \(\xi_\alpha = \sum_i \hat{v}_{ai} U_{ia}^\dagger z_a^*\), and noticing that \(\hat{v}_{ai} = \Omega - \hat{v}_i\), we finally have
\[ \langle \Psi | \Psi \rangle = \int \prod_{\alpha} \frac{d\xi_{\alpha}^\dagger d\xi_{\alpha}}{\pi} e^{-\xi^\dagger (\Omega - \hat{P})^{-1} \xi} \langle 0 | \prod_{\beta} (b_\beta)^{n_\beta} e^{\sum_{\alpha} \xi_{\alpha}^* \hat{b}_\alpha^\dagger} e^{\sum_{\alpha} \xi_{\alpha} b_\alpha} \prod_{\gamma} (b_\gamma^\dagger)^{n_\gamma} | 0 \rangle. \]  
(A.9)

Expanding the exponents and using the commutation relations, in particular the equality \(b^m b^m |0\rangle = (n!/(n - m)!)|b^{(n-m)}|0\rangle\) for \(m \leq n\), one can verify that
\[ \langle 0 | \prod_{\beta} (b_\beta)^{n_\beta} e^{\sum_{\alpha} \xi_{\alpha}^* \hat{b}_\alpha^\dagger} e^{\sum_{\alpha} \xi_{\alpha} b_\alpha} \prod_{\gamma} (b_\gamma^\dagger)^{n_\gamma} | 0 \rangle = \prod_{\alpha} \sum_{m=0}^{n_\alpha} \frac{(n_\alpha)!}{(m)!^2(n_\alpha - m)!} |\xi_{\alpha}|^{2m}, \]  
(A.10)
equal to \(\prod_{\alpha} n_\alpha! L^0_{n_\alpha} (-|\xi_{\alpha}|^2)\), using the definition of the generalized Laguerre polynomials, \(L^k_n(z) = \sum_{m=0}^n ((n+k)!/(m!)(k+m!)((n-m)!))(-z)^m\), which can be written also in terms of confluent hypergeometric functions, \(L^k_n(z) = ((k+n)!/(k!n!))(F_1(-n,k+1;z)\). As a final result, the norm of (A.1) can be written as an integral, equation (2), with the action
\[ S(\xi, \xi^\dagger) = \xi^\dagger (\Omega - \hat{P})^{-1} \xi - \sum_{\alpha} \ln [n_\alpha! L^0_{n_\alpha} (-|\xi_{\alpha}|^2)]. \]  
(A.11)

If \(n_\alpha = 1, \forall \alpha\), since \(L^0_{n_\alpha}(-|\xi_{\alpha}|^2) = (1 + |\xi_{\alpha}|^2)\), the action reduces to equation (3). The saddle point equation reads then
\[ \xi_\alpha = \sum_{\beta, n_\alpha > 0} (\Omega_{\alpha\beta} - \delta_{\alpha\beta}) \frac{L^1_{n_{\alpha} - 1} (-|\xi_{\beta}|^2)}{L^0_{n_\beta} (-|\xi_{\beta}|^2)} \xi_\beta, \]  
(A.12)

which reduces to equation (4), for all \(n_\alpha = 1\). Since, for \(|\xi_{\beta}|^2 \ll 1\), we can make the expansion \(L^k_n(-|\xi_{\beta}|^2) \simeq ((n+k)!/(n!k!))(1 + (n/(k+1))|\xi_{\beta}|^2)\), the eigenvalue equation, on discarding \(O(\xi_{\beta}^3)\) terms in the rhs of equation (A.12), becomes
\[ \xi_\alpha = \sum_{\beta} (\Omega_{\alpha\beta} - \delta_{\alpha\beta}) n_{\beta} \xi_\beta, \]  
(A.13)

which generalizes equation (5) for arbitrary \(n_{\beta}\).

**Appendix B: The reduced density matrix: two simple cases**

Here we are going to show within a toy model made up of two bosons arranged on three sites how disorder and interaction can conspire to enhance the bipartite entanglement entropy. With two bosons \(N = 2\) and without disorder, in the delocalized phase, \(|\xi_{\alpha}|^2 = 1/3\), from equations (38), (33), we get the following single-site entropy:
\[ S = 2 \ln 3 - \frac{16}{9} \ln 2 \simeq 0.96. \]  
(B.1)

DOI:10.1088/1742-5468/2011/08/P08004
What we shall be seeing in the following is that this value can be overcome by introducing a suitable amount of disorder.

If we now take equation (42) as the many-body wavefunction, we get, for \( N = 2 \) bosons and generic \( N_s \) sites, the following three diagonal elements of the reduced density matrix:

\[
\rho_0 = \frac{1}{\text{Per}(\Omega)} \sum_{i=2}^{N_s} \left( 2|\chi_{1i}\chi_{2i}|^2 + \sum_{j>i}^N |\chi_{1i}\chi_{2j} + \chi_{2i}\chi_{1j}|^2 \right) \]  

\( (B.2) \)

\[
\rho_1 = \frac{1}{\text{Per}(\Omega)} \sum_{i=2}^{N_s} |\chi_{1i}\chi_{2i} + \chi_{2i}\chi_{1i}|^2 \]  

\( (B.3) \)

\[
\rho_2 = \frac{2}{\text{Per}(\Omega)} |\chi_{1i}\chi_{2i}|^2. \]  

\( (B.4) \)

Let us now consider \( N_s = 3 \) and a simple on-site disorder such that \( \epsilon_i = \pm \Delta \). We can have therefore eight possible configurations of disorder. For \( U \gg \Delta \), by semiclassical considerations and using equations (B.2)–(B.4), we can have a probability \( \sim 1/4 \) of having \( S \simeq 0 \), i.e. \( P(S \simeq 0) \approx 1/4 \), while \( P(S \simeq \ln 2) \approx 1/2 \) and \( P(S \simeq 0.96) \approx 1/4 \), the same entropy as without disorder. For \( U \ll \Delta \), instead, we have \( P(S \simeq 0) \approx 1/2 \), \( P(S \simeq 0.96) \approx 1/4 \) and \( P(S \simeq \frac{3}{2}\ln 2 \approx 1.04) \approx 1/4 \), namely we can have a sizable probability of having maximum entropy for two bosons, and so exceeding the value in equation (B.1). The disorder, therefore, cause the probability distribution to peak at zero while widening the entropy fluctuations.

In general for filling \( \nu < 1 \), the superfluid single-site entropy is \( S \simeq \nu(1 - \ln \nu) \), as shown in the text. On introducing strong enough disorder, there is the possibility for a fraction \( k \) of the total sites to have very large local energies which make those sites inaccessible to the particles. This induces a larger effective filling, \( \nu/(1 - k) \), and consequently enhances the entropy.

For the sake of completeness we hereafter report the form of the reduced density matrix for \( N = 4 \) bosons, used in this paper in section 5.2. To simplify notation we define the matrix

\[
\mathcal{L}^{ijkl} = \begin{pmatrix}
\chi_{1i} & \chi_{1j} & \chi_{1k} & \chi_{1l} \\
\chi_{2i} & \chi_{2j} & \chi_{2k} & \chi_{2l} \\
\chi_{3i} & \chi_{3j} & \chi_{3k} & \chi_{3l} \\
\chi_{4i} & \chi_{4j} & \chi_{4k} & \chi_{4l}
\end{pmatrix}
\]  

\( (B.5) \)

in order that the single-site reduced density matrix can be written in the following form:

\[
\rho_0 = \frac{1}{\text{Per}(\Omega)} \sum_{i=2}^{N_s} \left\{ \sum_{j>i}^N \sum_{k>j}^N \sum_{l>k}^N |\text{Per}(\mathcal{L}^{ijkl})|^2 + \frac{1}{2!} \sum_{j>i}^N \sum_{k>i}^N \sum_{l>j}^N |\text{Per}(\mathcal{L}^{iijk})|^2 \\
+ \frac{1}{2!2!} \sum_{j>i}^N |\text{Per}(\mathcal{L}^{iij})|^2 + \frac{1}{3!} \sum_{j>i}^N |\text{Per}(\mathcal{L}^{iiij})|^2 + \frac{1}{4!} |\text{Per}(\mathcal{L}^{iiii})|^2 \right\} \]  

\( (B.6) \)

\[
\rho_1 = \frac{1}{\text{Per}(\Omega)} \sum_{i=2}^{N_s} \left\{ \sum_{j>i}^N \sum_{k>j}^N |\text{Per}(\mathcal{L}^{ijkl})|^2 + \frac{1}{2!} \sum_{j>i}^N |\text{Per}(\mathcal{L}^{iijk})|^2 + \frac{1}{3!} |\text{Per}(\mathcal{L}^{iiij})|^2 \right\} \]  

\( (B.7) \)

doi:10.1088/1742-5468/2011/08/P08004
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\[ \rho_2 = \frac{1}{\text{Per}(\Omega)} \sum_{i=2}^{N_s} \left\{ \frac{1}{2!} \sum_{j>i}^{N_s} |\text{Per}(L^{1ij})|^2 + \frac{1}{2!2!} |\text{Per}(L^{1ii})|^2 \right\} \]  \hspace{1cm} (B.8)

\[ \rho_3 = \frac{1}{\text{Per}(\Omega)} \frac{1}{3!} \sum_{i=2}^{N_s} |\text{Per}(L^{111i})|^2 \]  \hspace{1cm} (B.9)

\[ \rho_4 = \frac{1}{\text{Per}(\Omega)} \frac{1}{4!} |\text{Per}(L^{1111})|^2. \]  \hspace{1cm} (B.10)

From the equations above one can easily guess the form of the reduced density matrix for a generic value of \( N \).

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