Disordered Bosons: Condensate and Excitations

Kanwal G. Singh and Daniel S. Rokhsar

Department of Physics, University of California, Berkeley, California 94720

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Abstract

The disordered Bose Hubbard model is studied numerically within the Bogoliubov approximation. First, the spatially varying condensate wavefunction in the presence of disorder is found by solving a nonlinear Schrödinger equation. Using the Bogoliubov approximation to find the excitations above this condensate, we calculate the condensate fraction, superfluid density, and density of states for a two-dimensional disordered system. These results are compared with experiments done with $^4$He adsorbed in porous media.
I. INTRODUCTION

By definition, superfluids are robust to the introduction of weak microscopic disorder. A flowing superfluid is characterized by a macroscopic wavefunction whose phase varies across the sample; as long as this condensate wavefunction remains well defined, disorder cannot lead to the degradation of currents for topological reasons. With increasing disorder, however, the rigidity of the superfluid towards phase variations is reduced. For sufficiently large disorder superfluidity is eventually destroyed even at zero temperature, resulting in a Bose insulator (the “Bose glass”).

Disordered Bose condensates can be realized experimentally by superfluids in random media, such as $^4$He films adsorbed on porous Vycor glass. The first few monolayers of adsorbed $^4$He are not superfluid, even at low temperatures, and form an “inert” insulating layer of bosons localized by disorder. As the coverage is increased, a transition from this Bose insulator to a superfluid phase is observed. Crudely speaking, the first few monolayers are comprised of bosons occupying non-overlapping localized states, which screen the microscopic disorder of the porous glass for subsequently added bosons. Added bosons feel a smoother potential that is the sum of the initial random potential plus a Hartree repulsion from the localized particles. When the disorder is sufficiently well screened, condensation into an extended state occurs.

Of course, this picture is an oversimplification: the $^4$He atoms in the “inert” layer are indistinguishable from those in the condensate, and the true many-body wavefunctions must be completely symmetric with respect to particle interchange. Exchange between the “inert” and “condensed” bosons can be important, especially near the insulator-superfluid transition. The computational problem with this scheme is that, unlike the case of fermions, which by the exclusion principle must populate orthogonal states, bosons actually prefer to be in non-orthogonal states to optimize their effectively attractive exchange interactions. The need to symmetrize thwarts controlled general Hartree-Fock calculations.

We present here numerical calculations of the properties of highly disordered Bose
condensates using the Bogoliubov\textsuperscript{13} approximation, which has been formulated for disordered systems by Lee and Gunn\textsuperscript{14} and considered in the weak disorder limit by Meng and Huang.\textsuperscript{15,16} Although the Bogoliubov method is strictly valid only in the limit of weak repulsive interactions, we will consider strongly interacting systems as well (in the presence of arbitrary disorder) in an attempt to address the qualitative features of Bose systems in random media in a quasi-analytic fashion. Previous theoretical approaches include numerical simulations,\textsuperscript{17–20} scaling analysis,\textsuperscript{5} renormalization group calculations,\textsuperscript{3,21,22} and perturbative methods.\textsuperscript{23}

In the Bogoliubov approximation\textsuperscript{14} the disordered potential is screened by bosons occupying a delocalized condensate wavefunction which has larger amplitude where the random potential is deep. This non-uniform condensate is macroscopically occupied, and fluctuations into and out of it are considered due to residual interactions. These effects deplete the condensate non-uniformly, and lead to a spectrum of collective, phonon-like excitations.

The Bogoliubov scenario resembles the heuristic “inert layer” picture discussed above, but is constructed in the reverse order. \textit{First} the condensate is determined, and \textit{then} the (possibly localized) non-condensate part of the many-body wavefunction is considered. This localized, uncondensed part of the ground state corresponds to the “inert layer” discussed above, and can be crudely thought of as the zero temperature “normal” fluid excited from the condensate by disorder rather than thermal fluctuations (see Sec. VI for a more precise definition). The advantage of the Bogoliubov approach is that exchange between the “condensate” and the “normal” fluid is included naturally. Its disadvantage is that interactions within the normal fluid are essentially ignored.

The outline of this paper is as follows: In Section II, we introduce the disordered Hubbard model for bosons and in Section III we solve this model in the Hartree approximation. In Section IV we review the Bogoliubov approximation for disordered bosons. Sections V and VI present calculations of the depletion of the condensate and the reduction of the superfluid density due to disorder, respectively. Section VII reports calculations of the excitation spectrum and specific heat of the disordered condensate. Finally, in Section VIII
we summarize our results and discuss experiments.

II. THE BOSON HUBBARD MODEL

A simple model for disordered interacting bosons is the Hubbard model for lattice bosons in a random potential:

\[ \mathcal{H} = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \sum_i V(i) b_i^\dagger b_i + \frac{U}{2} \sum_i b_i^\dagger b_i^\dagger b_i b_i, \]

where \( b_i^\dagger \) (\( b_i \)) creates (destroys) a boson at lattice site \( i \). The sum on \( \langle i, j \rangle \) extends over all nearest-neighbor pairs of lattice sites, \( U \) is the strength of the repulsive on-site interaction, and \( t \) is a hopping matrix element. The random potential \( V(i) \) is uniformly distributed between \(-\Delta\) and \( \Delta \). The total number of bosons is \( \mathcal{N} \), and the number of lattice sites is \( \mathcal{V} \); the mean density is then \( n \equiv \mathcal{N} / \mathcal{V} \).

As a model for the behavior of \( ^4\)He adsorbed in Vycor on length scales less than the pore size (several hundred Ångströms), each site could represent a surface location of atomic dimension, connected to neighboring sites in a two-dimensional network. We will consider \( (\mathbb{II}) \) on two-dimensional square lattices of up to 306 sites, with periodic boundary conditions. To study disordered Bose condensates on longer length scales, the sites of model \( (\mathbb{II}) \) could themselves be used to represent pores in Vycor, with a three-dimensional connectivity. Since 300 sites is still quite a small three-dimensional lattice, we will only report calculations in two dimensions.

III. THE HARTREE CONDENSATE

A simple variational ground state for \( (\mathbb{II}) \) is the Hartree state

\[ \Psi(r_1, r_2, ..., r_N) = \phi_0(r_1)\phi_0(r_2)\ldots\phi_0(r_N), \]

where all bosons are condensed into the same real, normalized single-particle wavefunction \( \phi_0(i) \). The many-body state \( (\mathbb{II}) \) is explicitly symmetric under particle exchange, as befits
a Bose state. For a translationally invariant system, the single-particle state \( \phi_0(i) \) is independent of \( i \), and is simply the zero-momentum state. In a disordered system, this will no longer be the case: \( \phi_0(i) \) will adjust to be larger at the minima of the random potential and smaller at its maxima.

The expectation value of the Hamiltonian (1) in the variational state (2) is

\[
\langle \Psi | \mathcal{H} | \Psi \rangle = -tN \sum_{(i,j)} \phi_0(i) \phi_0(j) + N \sum_i V(i) \phi_0^2(i) + \frac{UN^2}{2} \sum_i \phi_0^4(i). \tag{3}
\]

To minimize (3) with respect to the (normalized) single particle state \( \phi_0 \) one must solve the discrete nonlinear Schrödinger equation

\[
- t \sum_{j=nn(i)} \phi_\lambda(j) + \tilde{V}(i) \phi_\lambda(i) = (\mu_0 + \epsilon_\lambda) \phi_\lambda(i), \tag{4}
\]

where the sum over \( j = nn(i) \) extends over the nearest neighbors \( j \) of site \( i \). The effective single-particle potential \( \tilde{V}(i) \) is given by

\[
\tilde{V}(i) \equiv V(i) + UN|\phi_0(i)|^2, \tag{5}
\]

where \( \phi_0(i) \) is the single particle ground state of (4).

For convenience, \( \mu_0 \) in eq. (4) is chosen so that \( \epsilon_0 \equiv 0 \), i.e., so that the Hartree excitation energies \( \epsilon_\lambda \) are measured with respect to the energy required to add a particle to the condensate. The condensate \( \phi_0(i) \) and the \( \mathcal{V} - 1 \) excited states denoted by \( \phi_\lambda(i) \) together form an orthonormal basis for single particle states. For convenience, sums over \( \lambda \) will always implicitly exclude the condensate.

We solve (4) and (5) iteratively, as follows. Beginning with a trial condensate \( \phi_0(i) \) (either the zero-momentum state or the exact state for \( t = 0 \)), we compute the corresponding screened potential \( \tilde{V}(i) \). The resulting single-particle Schrödinger equation is solved numerically to obtain a new set of single particle eigenstates. An improved trial condensate is then created by mixing the initial guess with the lowest energy eigenstate of the screened potential. This procedure is repeated until (4) and (5) are simultaneously satisfied. Simple
linear interpolation to obtain a new trial condensate converges very slowly, if at all. More rapid, consistent convergence was obtained with the Broyden mixing method commonly used in electronic structure calculations.\textsuperscript{23} Achieving convergence is the biggest obstacle in our calculation, particularly for large disorder, and limits the system sizes we can consider.

The condensate wavefunction $\phi_0(i)$ accumulates at the minima of the applied random potential, so that the screened potential $\tilde{V}(i)$ is smoother than $V(i)$, with shallower minima. These minima of the screened potential are more uniform than those of the original potential, with approximately the same depth. Roughly speaking, variations in the condensate conspire to create a screened potential which resembles the initial random potential, but with its deepest minima lopped off, as shown in Fig. 1. As the density $n$ (or the interaction strength $U$) is increased, the minima of $\tilde{V}(i)$ become shallower and shallower, since the screening is then more efficient. No long-range correlations are introduced in the screening process, as shown in Fig. 2.

To address the nature of the condensate and Hartree excited states, we calculate the participation ratio

$$P[\lambda] \equiv \frac{1}{\sum_i |\phi_\lambda(i)|^4}$$

of state $\lambda$, which measures the number of sites at which $\phi_\lambda(i)$ is appreciable.

The condensate wavefunction $\phi_0(i)$ is \textit{always} extended,\textsuperscript{2} and “participates” in a finite fraction of the lattice sites. The extended nature of the self-consistent ground state of (4) is demanded by the following argument: Assume that the state $\phi_0(i)$ were localized. Then for a non-vanishing density of bosons, macroscopically occupying this single-particle state as in (2) would confine a macroscopic number of interacting particles to a finite volume (the localization volume of $\phi_0(i)$). The interaction energy of the resulting many-body state would then vary as the square of the total particle number. In the thermodynamic limit, however, the total energy should be extensive. Thus the assumption of a localized $\phi_0(i)$ yields a contradiction, and the condensate must be extended.

This argument does not preclude a condensate wavefunction $\phi_0(i)$ which is “lumpy” –
i.e., one which is a (nodeless) superposition of well-separated, localized states. Strictly speaking, such a lumpy state is extended and the resulting Hartree state (2) is still a Bose condensate. We will see below that these lumpy condensates (found for strong disorder and weak repulsion) are particularly susceptible to depletion from scattering out of the condensate, and have substantially reduced superfluid densities. An alternative, and perhaps better, variational state could be constructed by instead placing a few particles in each of a large number of localized states. As these localized states overlap (they need not be orthogonal), however, it becomes difficult to calculate the energy and other properties of the properly symmetrized state. Unfortunately, the numerical tricks which enable efficient calculation with determinants fail for permanents.

It is well known that all eigenstates of a generic random potential in one and two dimensions are localized. How then can the condensate $\phi_0$ always be extended? The loophole that permits this is that the screened potential $\tilde{V}(i)$ is not generic, but has been tailored to the problem at hand specifically to produce an extended ground state. The condensate is not a “typical” state, but one whose peaks and valleys have been fed back into the disordered potential itself via (5). The extended nature of the condensate does not violate any accepted lore of localization.

An analysis of the participation ratio for (two-dimensional) systems ranging from $V = 72$ to $V = 306$ suggests that for small disorder, all states are extended (i.e., have a localization length larger than our largest system). Fig. 3 shows that the participation ratio scales with the size of the system. For sufficiently strong disorder, we find that the participation ratios of the Hartree excited states become independent of system size, indicating that they have all become localized. Only the condensate remains extended. It is interesting that the use of the self-consistent potential $\tilde{V}(i)$ converts the state of lowest energy (which in a typical single-particle localization problem would be the most localized state) to the unique extended state.
IV. THE BOGOLIUBOV APPROXIMATION

Given the self-consistent Hartree condensate, $\phi_0(i)$, we can proceed with the Bogoliubov approximation. Following Lee and Gunn, we expand the boson field operator $b_i$ in the complete set of operators $b_0$ and $\{b_\lambda\}$:

$$b_i = \phi_0(i)b_0 + \sum_\lambda \phi_\lambda(i)b_\lambda.$$  \hspace{1cm} (7)

Although interactions and the disordered potential will both deplete the condensate, in the Bogoliubov approximation this depletion is assumed to be small enough that the single-particle state $\phi_0(i)$ is still occupied by a macroscopic number $N_0$ bosons. To order $1/N_0$ we can then replace the creation and annihilation operators $b_0^\dagger$ and $b_0$ for this state by $\sqrt{N_0}$.

The total number of bosons in the system is the sum of those in the condensate and those not in the condensate:

$$N = N_0 + \sum_\lambda b_\lambda^\dagger b_\lambda.$$  \hspace{1cm} (8)

Expanding to first order in the depletion of the condensate, we then find

$$b_0 = \sqrt{N_0} = \sqrt{N} - \frac{1}{2\sqrt{N}} \sum_\lambda b_\lambda^\dagger b_\lambda + ...$$  \hspace{1cm} (9)

Inserting (7) and (9) into the disordered Hubbard model (1), and retaining all terms second order in $b_\lambda^\dagger$ and $b_\lambda$, yields

$$H_B = N\mu_0 - \frac{U N^2}{2} \sum_i |\phi_0(i)|^4 + \sum_{\lambda\lambda'} \epsilon_\lambda b_\lambda^\dagger b_\lambda + \sum_{\lambda\lambda'} S_{\lambda\lambda'} (b_\lambda^\dagger b_{\lambda'} + b_\lambda^\dagger b_\lambda + b_{\lambda'}^\dagger b_{\lambda'} + b_{\lambda'} b_\lambda).$$  \hspace{1cm} (10)

The first line of (10) specifies the single-particle and self-interaction energies of the condensate, and the energy $\epsilon_\lambda$ for adding a particle in the excited state $\lambda$. The second line involves the inner product

$$S_{\lambda\lambda'} \equiv \sum_i \phi_\lambda(i)|\phi_0(i)|^2 \phi_{\lambda'}(i).$$  \hspace{1cm} (11)
of states $\lambda$ and $\lambda'$ weighted by the condensate density, which gives the amplitude for (a) single-particle scattering by the condensate and (b) pair scattering into and out of the condensate. Since the condensate is non-uniform, these scattering processes will generally not conserve momentum.

To arrive at (10) terms cubic and higher order in field operators $b_\lambda$ and $b_\lambda^\dagger$ have been discarded. This is equivalent to the random phase approximation, and includes interactions between the non-condensate bosons and the condensate while neglecting interactions among the uncondensed bosons. These approximations are controlled in the dilute, weakly interacting limit in which the condensate fraction $N_0/N$ is close to unity (see Sec. V). Here we will push the Bogoliubov approximation to its limits, and hope that the qualitative results are representative of disordered Bose condensates.

The quadratic Hamiltonian (10) can be diagonalized by canonical transformation to a set of quasiparticle creation and annihilation operators $\gamma^\dagger$ and $\gamma$ such that

$$[H_B, \gamma^\dagger_\mu] = \omega_\mu \gamma^\dagger_\mu,$$

where $\omega_\mu$ is the quasiparticle excitation energy. This transformation is accomplished by taking linear combinations of creation and annihilation operators:

$$\gamma^\dagger_\mu = \sum_\lambda \left( u_{\mu\lambda} b_\lambda^\dagger + v_{\mu\lambda} b_\lambda \right).$$

Like the index $\lambda$ labeling the Hartree states, the index $\mu$ labeling quasiparticle states runs from 1 to $V - 1$.

To satisfy (12), the coefficients $u_{\mu\lambda}$, $v_{\mu\lambda}$ must obey the generalized eigenvalue equation

$$\begin{pmatrix} A_{\lambda\lambda'} & -B_{\lambda\lambda'} \\ -B_{\lambda\lambda'} & A_{\lambda\lambda'} \end{pmatrix} \begin{pmatrix} u_{\mu\lambda'} \\ v_{\mu\lambda'} \end{pmatrix} = \omega_\mu \begin{pmatrix} \delta_{\lambda\lambda'} & 0 \\ 0 & -\delta_{\lambda\lambda'} \end{pmatrix} \begin{pmatrix} u_{\mu\lambda'} \\ v_{\mu\lambda'} \end{pmatrix},$$

where
\[ A_{\lambda\lambda'} \equiv \epsilon_{\lambda} \delta_{\lambda\lambda'} + UNS_{\lambda\lambda'}, \]
\[ B_{\lambda\lambda'} \equiv UNS_{\lambda\lambda'}. \]  
(Summation over the repeated index \( \lambda' \) is implied.) Note that if \( (u^v) \) is a solution with excitation energy \( \omega \) (corresponding to \( \gamma^\dagger \)), then \( (v^u) \) is a solution with \(-\omega\) (corresponding to \( \gamma \)). The orthonormality conditions
\[ \begin{pmatrix} u_{\mu\lambda} & u_{\mu\lambda} \end{pmatrix} \begin{pmatrix} \delta_{\lambda\lambda'} & 0 \\ 0 & -\delta_{\lambda\lambda'} \end{pmatrix} \begin{pmatrix} u_{\mu'\lambda'} \\ v_{\mu'\lambda'} \end{pmatrix} = \delta_{\mu\mu'} \]  
are automatically satisfied by normalized solutions of (14), and guarantee that the quasiparticle operators \( \gamma^\dagger_\mu \) obey Bose commutation relations: \([\gamma_\mu, \gamma^\dagger_{\mu'}] = \delta_{\mu\mu'} \) and \([\gamma_\mu, \gamma_{\mu'}] = 0 \).

The ground state energy \( E_G \) in the Bogoliubov approximation is
\[ E_G = N\mu_0 - \frac{UN^2}{2} \sum_{\lambda} |\phi_0(i)|^4 \]
\[ + \sum_{\lambda\lambda'} \left[ (\epsilon_{\lambda\lambda'} + UNS_{\lambda\lambda'}) u_{\mu\lambda} v_{\mu\lambda'} - UNS_{\lambda\lambda'} u_{\mu\lambda} v_{\mu\lambda'} \right]. \]
The last line gives the zero-point contribution of the quasiparticle modes.

**V. THE CONDENSATE FRACTION**

The ground state wavefunction \( |G\rangle \) in the Bogoliubov approximation is the state annihilated by all of the quasiparticle destruction operators \( \gamma_\mu^\dagger \):
\[ |G\rangle = (b_0^\dagger)^{N_0} \Pi_{\lambda\lambda'} \exp[-M_{\lambda\lambda'} b_\lambda^\dagger b_{\lambda'}^\dagger] |\text{vac}\rangle, \]
where \( |\text{vac}\rangle \) is the state with no bosons and \( M_{\lambda\lambda'} \) is defined implicitly by
\[ \sum_{\lambda} u_{\mu\lambda} M_{\lambda\lambda'} = v_{\mu\lambda}. \]
The number of particles in the condensate, \( N_0 \), is determined by calculating the mean number of bosons *not* in the condensate \( \sum_{\lambda} b_\lambda^\dagger b_\lambda \) and subtracting it from the total particle number (see eq. (8)).
In a translationally invariant system, the condensate fraction measures the occupation of the zero-momentum state. In a disordered system, the proper definition of the condensate fraction is the largest eigenvalue of the one particle density matrix \( 26 \) The condensate density is then given by the square of the off-diagonal long-range order parameter:

\[
\lim_{|i-j| \to \infty} \langle G | b_i^\dagger b_j | G \rangle = \langle G | b_i^\dagger | G \rangle \langle G | b_j | G \rangle = N_0 \phi_0(i) \phi_0(j). \quad (20)
\]

Fig. 4 shows the condensate fraction, \( N_0 / N \), as a function of disorder for several values of the interaction strength. The calculation is done by averaging over 7 realizations of disorder on \( L_x \times L_y \) lattices where \( L \) ranges from 8 to 18. We then extrapolate to the thermodynamic limit. Even in the absence of disorder, particles are scattered out of the condensate as a result of their mutual interactions, and \( N_0 / N \) is less than unity. For weak disorder, the number of bosons in the condensate stays roughly fixed, while the condensate wavefunction itself is distorted to accommodate the random potential.

This insensitivity of the condensate fraction to weak disorder is a crude criterion for superfluidity, although the proper quantity to consider is the superfluid density (see below). Fig. 4 shows that as the interaction strength \( Un/t \) increases, the system becomes more robust to the addition of disorder, so that larger values of \( \Delta \) are required to further deplete the condensate beyond the effect of interactions alone.

At large values of disorder, the condensate fraction drops to zero. As the condensate fraction becomes small, the approximation of truncating the Bogoliubov Hamiltonian \( 10 \) at quadratic order becomes worse and worse, and our calculations cannot be considered quantitative. Nevertheless, our calculation suggests that for sufficiently high disorder the condensate is destroyed, and a “Bose glass” is reached. Although the logic leading to it breaks down for \( N_0 = 0 \), the Bogoliubov ground state \( 18 \) with vanishing condensate density is a potentially useful variational state for the Bose glass.

In the Hartree calculation of Sec. II, the applied random potential \( V(i) \) is screened by \( NU | \phi_0(i) |^2 \), which is equivalent to assuming that all of the bosons are in the condensate.
As the condensate is depleted, does this estimate of the screened potential continue to hold? To check this, we compare the ground state expectation value of the boson density at site \( i \), \( \langle G | b_i^\dagger b_i | G \rangle \), with the density obtained in the Hartree approximation, \( \mathcal{N} | \phi_0(i) |^2 \). As Fig. 3 shows, the density in the Bogoliubov approximation faithfully tracks the density in the Hartree approximation. Even when the condensate is significantly depleted, the particles scattered from it remain in their original vicinity, and continue to screen the initial random potential as if they had remained in the condensate.

VI. SUPERFLUID DENSITY

The superfluid density of a Bose condensate distinguishes between the low-frequency, long-wavelength transverse and longitudinal responses of the system. (This quantity should not be confused with the condensate fraction discussed above, which is a ground state expectation value that measures the degree of off-diagonal long-range order.) A longitudinal probe corresponds to boosting the system, and the entire fluid responds. A low-frequency transverse probe corresponds to a slow rotation of the system, which only couples to the normal fluid, leaving the superfluid untouched. The superfluid density is defined simply as the difference between the longitudinal and transverse response. In principle, a Bose system can be superfluid without possessing true off-diagonal long-range order, the canonical example being the two-dimensional Bose liquid at non-zero temperature below the Kosterlitz-Thouless transition, which has only algebraic correlations.

The zero-temperature, zero-frequency, current-current response tensor \( \chi_{ij}(q, \omega = 0) \) is given by the Kubo formula\(^{27}\)

\[
\chi_{ij}(q, \omega = 0) \equiv -2 \sum_m \frac{\langle G | J_j(q) | m \rangle \langle m | J_i(q) | G \rangle}{\omega_m}.
\]

The sum extends over all intermediate excited states \( m \), and the lattice current operator \( J(q) \) is defined by

\[
J_i(q) = 2t \sum_k \sin(k_i + \frac{q_i}{2}) b_k^\dagger b_{k+q}.
\]
where \( b_k = \sum_i e^{i k \cdot r_i} b_i \). In principle the direct evaluation of \( \chi_{ij} \) is straightforward given a complete knowledge of the excited states \( |m\rangle \).

In the continuum, the longitudinal response in the long wavelength limit is required by the the \( f \)-sum rule to satisfy

\[
\lim_{q \to 0} \chi_{xx}(q \hat{x}) = -2tN,
\]

i.e., the entire fluid participates in longitudinal flow. On a lattice, the \( f \)-sum rule is modified so that

\[
\lim_{q \to \infty} \chi_{xx}(q \hat{x}) = -2tN_{\text{eff}} = -2t[N - \sum_k \epsilon_k \langle n_k \rangle],
\]

where \( \epsilon_k \) is the tight-binding dispersion given below in (30). (This sum rule holds in the presence of arbitrary disorder.) Eq. (24) implicitly defines \( N_{\text{eff}} \). Even though \( N_{\text{eff}} \neq N \), the longitudinal response of a lattice system still corresponds to the entire fluid.

The transverse response of a Bose liquid is only due to the “normal fluid,” since the superfluid component of the system can only participate in irrotational (i.e., longitudinal) flow. Thus we can define the number of bosons in the normal fluid, \( N_n \), by

\[
\lim_{q \to 0} \chi_{xx}(q \hat{y}) \equiv -2tN_n.
\]

This definition also holds in the continuum, with \( t \) replaced by \( \hbar^2/2m \).

In a non-superfluid system, the long-wavelength longitudinal and transverse responses are identical. Superfluidity occurs when the two responses become different. The superfluid (number) density \( n_s \) is then defined by the difference between the longitudinal and transverse response, per unit volume:

\[
n_s = \frac{N_s}{V} = \frac{N_{\text{eff}} - N_n}{V}.
\]

The longitudinal and transverse response functions \( \chi_{xx}(q \hat{x}) \) and \( \chi_{xx}(q \hat{y}) \) can be easily calculated numerically in the Bogoliubov approximation. The excited states \( |m\rangle \) entering (21) are then all one and two quasiparticle states. Because the Bogoliubov approximation

\[13\]
does not conserve particle number, the lattice $f$-sum rule (24) is not satisfied. Explicit evaluation of (21) shows that $\lim_{q \to \infty} \chi_{xx}(q \hat{x})$ tends to the number of bosons in the condensate, $N_0$, rather than the total particle number $N$ (Note that $N_0$ is not the same as $N_{\text{eff}}$ in (24).)

The normal fluid density, obtained by explicit calculation in the Bogoliubov approximation of the transverse response function $\chi_{xx}(q \hat{y})$, appears to be more trustworthy. $N_n$ vanishes in the translationally invariant case ($V(i) = 0$), as expected. We therefore follow ref. 15 and adopt (26) as our operational definition of the superfluid density in the Bogoliubov approximation.

Fig. 6 shows the transverse response function for a $12 \times 13$ lattice averaged over 6 realizations of various weak disorder. Such small systems were used because the evaluation of the response tensor $\chi_{ij}(q, \omega = 0)$ in the presence of disorder requires four nested sums over quasiparticle states for each $q$ and is computationally very expensive. Fig. 6 shows $N_{\text{eff}}$ and $N_n$ for the same systems. $N_{\text{eff}}$ is calculated by explicitly evaluating the right hand side of (24), whereas $N_n$ is obtained from extrapolating the transverse response from Fig. 6 to $q = 0$. The difference between $N_{\text{eff}}$ and $N_n$ is $N_s$. For weak disorder ($\Delta/t < 5$), the fluctuations from realization to realization are small. With increasing disorder, however, these fluctuations become quite large, as seen by the error bars in Fig. 6 which represent sample-to-sample fluctuations. Note that the zero-frequency transverse response shows little dependence on momentum in this approximation.

An alternative definition of superfluid density is as a stiffness to variations in the phase of the condensate wavefunction [2]. Such a phase variation imposes a superfluid velocity on the system,

$$v_s = \frac{\hbar}{m} \nabla \theta,$$

(27)

where $\theta$ is the phase of the condensate wavefunction. The total energy of the system increases due to the kinetic energy of the superflow, and is directly proportional to the density of superfluid. The superfluid density is then defined by

$$\frac{\Delta E}{V} = \frac{\hbar^2 \rho_s}{2m^2} (\nabla \theta)^2.$$

(28)
It is easy to estimate the superfluid density in this manner using the energy of the Hartree state $\langle 2 \rangle$. (In principle, one should also include the change in the zero-point energy of the quasiparticles $\langle 17 \rangle$, but this calculation is also costly.) To impose a twist in boundary conditions, we should change the hopping matrix elements $t_{ij}$ to $t_{ij}e^{iA_{ij}}$, where $A_{ij}$ is a vector potential whose sum along a path spanning the sample is $\theta$. We should then solve the corresponding new non-linear Schrodinger equation, and compare the resulting condensate energies. Unfortunately, for $\theta \neq n\pi$ this requires solving a complex non-linear Schrodinger equation.

For $\theta = \pi$, the Schrodinger equation $\langle 4 \rangle$ remains real, but a new problem arises. Consider first the uniform case with $V(i) = 0$. With a $\pi$ phase twist, the ground state manifold of $\langle 4 \rangle$ is doubly degenerate, and is spanned by the uniformly left- and right-moving condensates. This degeneracy frustrates our iterative convergence scheme, since linear combinations of these two degenerate solutions have spatially varying densities, driving even the Broyden method away from convergence. This problem persists in the disordered case.

To avoid these complications, we note that for a phase difference of $\theta = 2\pi$ the Schrodinger equation is unchanged. In the course of increasing the phase difference from 0 to $2\pi$, the ground state is deformed into the first excited state. Thus we have taken the energy $\epsilon_{\lambda=1}$ of the first Hartree excited state in the absence of a twist to be the energy for introducing a $2\pi$ phase twist across the sample. In our problem, the superfluid density can then be computed by

$$\frac{N\epsilon_1}{V} = 2\rho_s t^2 \left(\frac{2\pi}{L}\right)^2.$$  (29)

(Strictly speaking, $N_{\text{eff}}$ should be used in place of $N$ in (29), since without disorder the normal fluid density vanishes, while the longitudinal response is given by $N_{\text{eff}}$. This correction is comparable in magnitude to the alteration of the zero-point motion of the quasiparticle energy, which we have also neglected in obtaining (29).)

Fig. 8 shows the superfluid fraction obtained using (29) and again extrapolating to the thermodynamic limit by averaging over 7 realizations for system sizes from $L = 8$ to
18. For weak disorder, when the direct evaluation of the response function permits reliable extrapolation to $q = 0$, the two calculations agree. As the disorder grows, however, the fluctuations in the response function \( \chi_{ij} \) from sample to sample increase, and beyond $\Delta/t \sim 10$ the direct calculation of $\chi_{ij}$ is no longer feasible because of the large number of samples required to obtain a reasonable statistical average.

As shown in Fig. 8, systems with larger interaction are more robust to the addition of disorder and thus require larger $\Delta$ to reduce the superfluid density. (This was also the case with the condensate fraction; compare with Fig. 4.) In fact, the superfluid fraction remains substantial even when the Bogoliubov approximation begins to break down, \textit{i.e.}, when the condensate fraction becomes small. Note that the superfluid response involves both the bosons in the condensate and those that have been scattered out of it by interactions – when the condensate is accelerated, some of these scattered bosons accompany it. In the absence of disorder (and neglecting lattice effects\(^\text{29}\)) all bosons participate, and $\rho_s = \rho$, even though the condensate can be substantially depleted. As $Un/t$ is increased for fixed disorder, the condensate fraction $N_0/N$ is reduced (because of increased scattering out of the condensate), while the superfluid fraction $\rho_s/\rho$ is increased (because of decreased sensitivity to disorder when interactions are strong).

\section*{VII. EXCITATION SPECTRUM}

At long wavelengths, the collective excitations of a uniform Bose condensate are phonons with a linear dispersion, $\omega = ck$. For wavelengths comparable to the interparticle spacing, strongly interacting Bose fluids exhibit a roton minimum, and for even shorter wavelengths the collective excitations become ill defined, merging with the multiparticle continuum\(^\text{27}\).

In the Bogoliubov approximation for lattice bosons without disorder, the quasiparticle spectrum can be solved analytically. The tight-binding dispersion is

$$
\epsilon_k = -2t[\cos(k_x) + \cos(k_y) - 2],
$$

and quasiparticle dispersion is
\( \omega_k = \sqrt{2Un\epsilon_k + \epsilon_k^2}. \) (31)

A linear phonon dispersion holds for wavelengths that are long enough that (a) \( \epsilon_k \) is much less than \( t \), so that the tight-binding dispersion is nearly quadratic \( (\epsilon_k \approx tk^2) \), and (b) \( \epsilon_k \) is much less than \( 2Un \), so that the first term in the square-root in (31) dominates. The speed of sound \( c \) is then \( \sqrt{2Un}t \).

The Bogoliubov approximation is too crude to capture the roton minimum found in real strongly-interacting Bose fluids, and for higher momenta the excitation energy (31) rises monotonically. At short wavelengths pair scattering can be neglected, and the quasiparticles behave as free particles with a Hartree energy \( \omega_{HF} = tk^2 + Un \).

When disorder is introduced, translational invariance is destroyed, and momentum is no longer a good quantum number. Are the excitations created by \( \gamma_\mu^\dagger \) localized? Even if the Hartree states \( \phi_\lambda \) are localized, the quasiparticle states created by \( \gamma_\mu^\dagger \) need not be – the condensate is extended, and can mediate non-local scattering via the inner product \( S_{\lambda\lambda'} \) in the Bogoliubov Hamiltonian (10).

Since the quasi-particle operators \( \gamma_\mu^\dagger \) do not simply add a boson, but superpose a particle and a “hole” (a particle supplied by the condensate), the participation ratio used for the Hartree excitations (eq. (3)) is inappropriate. Transforming (13) to the site basis, the quasiparticles are created by

\[
\gamma_\mu^\dagger = \sum_i (U_\mu_i b_i^\dagger + V_\mu_i b_i).
\] (32)

Adding an excitation in state \( \mu \) to the ground state, there is amplitude \( U_{\mu i} \) to create a particle at site \( i \) and \( V_{\mu i} \) to create a “hole” there. The net particle density at site \( i \) in the one quasiparticle state \( \gamma_\mu^\dagger |G\rangle \) differs from the density of the ground state itself by

\[
\delta n_{\mu i} \equiv \langle G | \gamma_\mu n_i \gamma_\mu^\dagger |G\rangle - \langle G | n_i |G\rangle = |U_{\mu i}|^2 + |V_{\mu i}|^2.
\] (33)

The corresponding “participation ratio” specifying the degree of delocalization of this density fluctuation is then
\[ P[\mu] = \frac{\left( \sum_i \delta n_{\mu i} \right)^2}{\sum_i \delta n_{\mu i}^2}. \] (34)

For an extended excitation, the participation ratio \( P[\mu] \) should scale linearly with the volume of the system; for a localized excitation, the participation ratio should become independent of the volume for systems larger than the localization length. Unfortunately, we could not perform a reliable scaling analysis with the small systems available to us, and we therefore could not infer the nature of the excitations created by \( \gamma^\dagger_\mu \). On general grounds, however, we expect the nature of the excitations in a disordered Bose condensate to be given by the localization problem for phonons. Thus in two dimensions, all excitations should be localized with a frequency dependent localization length \( \xi(\omega) \sim \exp[A/\omega^2] \) for arbitrary disorder. (In three dimensions, a mobility edge separates the extended low energy phonons from higher energy localized modes.)

Within the Bogoliubov approximation (10), the excited states of the system are independent bosons created by \( \gamma^\dagger_\mu \). If we assume that the temperature is low enough that thermal fluctuations do not change the excitation spectrum appreciably, but merely excite the quasiparticle states according to the Bose-Einstein distribution, the specific heat is then completely determined by the density of quasiparticle states per unit energy. For a density of states \( g(\omega) \), the specific heat is

\[
\frac{C(T)}{k_B} = \int_0^\infty \frac{\omega^2}{(k_B T)^2} \frac{g(\omega)e^{\omega/k_BT}}{[e^{\omega/k_BT} - 1]^2} d\omega.
\] (35)

To infer the behavior of the specific heat at low temperatures, it is useful to introduce the “integrated density of states”

\[
N(\omega) \equiv \int_0^\omega g(\omega')d\omega' = \sum_\mu \Theta(\omega - \omega_\mu),
\] (36)

where \( \Theta(\omega) \) is the Heaviside step function. \( N(\omega) \) gives the number of states with energy less than or equal to \( \omega \). As a monotonic function of \( \omega \), \( N(\omega) \) is easier to fit than the spiky \( g(\omega) \) for finite systems. If \( N(\omega) \sim \omega^x \), then \( C(T) \sim T^x \) for low temperatures. For a linear phonon dispersion \( \omega = ck \) in a \( d \)-dimensional box of linear dimension \( L \), the integrated density of
states varies as \( N(\omega) \sim (L\omega/c)^d \), so that the specific heat of a uniform Bose condensate varies as \( T^d \) at low temperatures.

For the finite \( L_x \times L_y \) lattices we consider, the momenta \( \mathbf{k} \) are restricted to a discrete set of allowed values. Only a limited number of these values satisfy the condition that \( \epsilon_\mathbf{k} \) be much smaller than both \( t \) and \( 2Un \) (or equivalently, that \( \omega \) be much smaller than both \( \sqrt{2Un}t \) and \( 2Un \)) needed for (30) and (31) to yield the correct linear dispersion in the absence of disorder. To obtain enough states to permit a fit to the density of states in this regime, we are forced to work with large \( Un \) even though the Bogoliubov approximation is uncontrolled in this limit. The condition that \( \epsilon_\mathbf{k} \) is much less than \( t \) guarantees that we avoid the van Hove singularity at the center of the tight-binding band. (The van Hove singularity can also be pushed to higher energy by the judicious addition of further range hopping matrix elements which cancel the \( k^4 \) terms in (31) and prolong the \( k^2 \) dependence of \( \epsilon_\mathbf{k} \).)

In the presence of disorder, the low energy integrated density of states will deviate from its pure \( \omega^d \) form. The integrated density of states divided by \( \omega^2 \) is shown for increasing disorder in Fig. 9. Each panel shows \( N(\omega)/\omega^2 \) for one realization of disorder. The low-energy end of the spectrum (well below the van Hove singularity, and in the range which had a linear dispersion in the absence of disorder) is well-fit by

\[
N(\omega) = A\omega + B\omega^2,
\]

where \( A \) and \( B \) depend on both \( \Delta/t \) and \( Un/t \).

Fig. 10 shows the parameters \( A \) and \( B \) vs. disorder for \( Un/t = 3.3 \). (Qualitatively similar behavior is found for \( Un/t = 5.0 \) and \( 7.0 \).) For weak disorder the integrated density of states remains nearly quadratic in \( \omega \), consistent with the low energy excitations being weakly perturbed phonons. As disorder increases, however, a linear contribution to \( N(\omega) \) emerges, corresponding to a constant density of states \( g(\omega) \). By the time the condensate is nearly completely depleted, the linear contribution to \( N(\omega) \) dominates.
Gillis et al. have measured the low temperature (50 mK - 1 K) heat capacity of thin $^4$He films adsorbed in porous Vycor glass. At low coverages, they find that the heat capacity is linear, with no evidence of a superfluid transition. This phase is identified with the insulating state of bosons localized by disorder, the “Bose glass.” Above a critical coverage (corresponding to several monolayers), the low temperature phase is a superfluid, with a heat capacity that varies as $T^2$.

Although the $^4$He is adsorbed as a few-monolayer film in the Vycor, the pores are connected to form a three-dimensional network. For sufficiently long wavelengths, three-dimensional behavior is expected. Why does the specific heat of the superfluid vary as $T^2$ rather than $T^3$, as expected for a three-dimensional condensate? The explanation is that for excitations with wavelengths less than the typical pore size $\lambda_{\text{pore}}$ (several hundred Ångströms), the connectivity of the porous network is unimportant, and the density of states for phonon-like excitations will be that of a two-dimensional superfluid. Thus above a crossover temperature $k_B T_x \sim \hbar c/\lambda_{\text{pore}}$, the specific heat should vary as $T^2$, until the roton contribution becomes appreciable. For an upper bound on $T_x$ we can use the bulk speed of sound $c \sim 3 \times 10^4$ cm/sec, which gives a crossover temperature of 30 mK. This is surely an overestimate, since at the coverages studied by Gillis et al. the pores are not close to being filled and the compressibility is therefore much less than in bulk. An alternative estimate using the speed of sound in thin $^4$He films adsorbed on graphite gives a crossover temperature of 1 mK.

How big a linear specific heat does one expect in the Bose glass? If one assumes a constant density of bosonic excitations in the Bose glass (as we found for the strongly disordered superfluid), then the observed linear specific heat translates to roughly one mode per particle per 10 $\mu$eV. This energy scale is comparable to the quantum confinement energy of a $^4$He atom trapped in a pore several hundred Ångströms in diameter.

We have presented numerical solutions of the disordered Bose Hubbard model in the Bo-
goliubov approximation. This approximation correctly captures the long wavelength properties of the clean Bose condensate, and is equivalent to the random phase approximation. It represents an expansion about the weakly disordered and weakly interacting limit, with a small parameter given by the depletion of the condensate. We find that weak disorder hardly affects the condensate fraction or the superfluid density. Instead, the condensate distorts to screen the imposed random potential. Interactions help stabilize the condensate, and prevent its collapse into a macroscopically occupied localized state.

For strong disorder the condensate fraction and superfluid density are reduced, and ultimately vanish for sufficiently large disorder (although the Bogoliubov approximation is no longer controlled by this point). Our calculation therefore cannot access the critical properties of the superfluid-insulator transition. The Bogoliubov calculation, however, does suggest a promising variational state for the Bose glass.

The clean Bose condensate has a linear low energy density of states in two dimensions, which implies a low temperature specific heat that varies as $T^2$, as observed. We find that with increasing disorder a constant density of states appears at low energy. This constant density of states dominates as the condensate fraction and superfluid density become small, and leads to a linear low temperature specific heat. With our small sample sizes, we could not determine the extent to which these excitations are localized.

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FIGURES

FIG. 1. The condensate wavefunction $\phi_0$ is concentrated at the minima of the “bare” potential $V(i)$. The effective potential felt by the bosons is therefore increased in the regions of high condensate density, so that the resulting self-consistently determined potential $\tilde{V}(i)$ resembles the original potential $V(i)$ with its lowest values lopped off. (Here $Un/t = 3.3$ and $\Delta/t = 10.0$)

FIG. 2. The autocorrelation function of the screened potential. Note that the screened potential does not develop any long-range correlations. ($\mathcal{V} = 210$ sites and $Un/t = 3.3$)

FIG. 3. An example of the participation ratio for the Hartree quasiparticle states $\phi_\lambda$ as a function of their energy $\epsilon_\lambda$ for several system sizes. ($Un/t = 3.3$ and $\Delta/t = 10.0$)

FIG. 4. The condensate fraction $N_0/N$ versus disorder $\Delta/t$ for several interaction strengths, extrapolated to $\mathcal{V} \to \infty$.

FIG. 5. The density $\langle G|n_i|G \rangle$ of the Bogoliubov ground state versus the density $\mathcal{N}|\phi_0(i)|^2$ of the Hartree state. Note that despite the large depletion of the condensate in the Bogoliubov state, the total density is well approximated by the density of the completely condensed state. ($Un/t = 3.3$)

FIG. 6. The transverse component of the current-current response function for the $12 \times 13$ lattice. ($Un/t = 3.3$)

FIG. 7. $N_{\text{eff}}/N$ and $N_n/N$ vs. disorder for the $12 \times 13$ lattice. $N_s = N_{\text{eff}} - N_n$. ($Un/t = 3.3$)

FIG. 8. The superfluid fraction as obtained through the twist method for several interaction strengths, extrapolated to $\mathcal{V} \to \infty$.

FIG. 9. $N(\omega)/\omega^2$ vs. $\omega$ for $Un/t = 3.3$ and (a)$\Delta/t = 0.0$ (b)$\Delta/t = 10.0$ (c)$\Delta/t = 18.0$. As disorder increases, $N(\omega)/\omega^2$ diverges, indicating a deviation from the form $N(\omega) \sim \omega^d$. ($\mathcal{V} = 210$ sites.)
FIG. 10. Coefficients of the linear and quadratic parts of the integrated density of states $N(\omega) = A\omega + B\omega^2$ vs. disorder (210 site system). As disorder is increased, the linear term develops, indicative of a glassy system.