Mean-Field Theory of the Localization Transition of Hard-Core Bosons

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A mean-field theory of the localization transition for strongly interacting bosonic systems is developed. Localization is shown to be sensitive to the distribution of the random site energies. It occurs in the presence of a triangular distribution, but not a uniform one. The inverse participation ratio, the single site Green's function, the superfluid order parameter, and the corresponding susceptibility are calculated, and the appropriate exponents determined. All of these quantities indicate the presence of a new phase, which can be identified as the *Bose glass*.

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The localization transition in disordered systems has been a focus of statistical and condensed matter physics ever since the famous paper of Anderson [1]. Though most of the work deals with the metal-insulator transition in fermionic systems, there is a recent surge of interest in bosonic models [2,3]. The superconductor-insulator transitions in granular superconductors [4] or ^{4}He in disordered media [5] are the paradigmatic experimental realizations of such systems. The theoretical understanding of phase transitions is typically based on a mean-field description and subsequent fluctuation analysis. The generally held belief even today is that the spatial homogeneity of this "mean field" allows only for extended states, thus obliterating the localized phase [2]. Below we demonstrate that in a model of hard-core bosons with random site energies and infinite range hopping this conventional wisdom does not hold, and with a suitable choice of the disorder distribution the localization transition can indeed be captured within the mean-field technique.

To highlight the involved physics, consider the standard argument against a transition in infinite connectivity lattices. It is believed [2] that because of the infinite number of neighbors every site will be connected to "virtually degenerate" sites for a continuous distribution of the disordered site energies. Thus hopping between these sites *always* gains kinetic energy with no cost in potential energy, delocalizing the particles. We argue that this simplified picture does not hold. To see this let us observe that for a finite system of size N, the gain from hopping between two sites is $\mathcal{O}(1/N)$, and the potential energy difference to the energetically closest sites is of the same order, since one has N site energies chosen independently from a finite interval. This means that there is a finite probability that for a given site *no sites at all* are available within the $1/N$ energy window set by the kinetic energy. When hopping from such a site, the potential energy cost certainly outweighs the kinetic energy gain. A complex sum of gains and costs will decide whether a state will be localized or extended. As shown quantitatively below, a wave function localized on energetically favorable sites will have only $\mathcal{O}(1/N)$ amplitudes on the rest of the sites, due to the scale of the hopping. Though there are $\mathcal{O}(N)$ such small amplitude sites, their contributions vanish in the thermodynamic limit.

For a reference frame, consider the spectrum of the ordered array. The ground state is homogeneous, nondegenerate with an energy of -1, clearly maximally benefiting from the kinetic term. *All* of the other $N-1$ single particle excited states possess zero energy. This is so because in this model to ensure orthogonality to the ground state the wave functions of the excited states have fluctuating signs across the sample. This *destructive quantum interference* frustrates the kinetic term, preventing any gain from the hopping process. So for weak disorder there is more kinetic energy to be gained by staying extended, and only a sufficiently strong disorder can localize the ground state. For the excited states, however, staying localized at a suitable site offers the lowering of the total energy in the absence of a kinetic energy premium, thus the excited states will become localized for *arbitrarily small disorder*. As we will see, this physics can be brought out by a nontraditional choice of the disorder: we will focus on the triangular distribution of the site energies.

As we want to develop a mean-field description of the localization transition, we consider the Hamiltonian with infinite range hopping, where this approach is exact,

$$H = -\sum_{i,j} J_{ij} a_i^\dagger a_j , \tag{1}$$

where $a_i^\dagger$ (a_i) creates (annihilates) a hard-core boson at site i ($i = 1, \ldots, N$), i.e., $a_i^\dagger a_i + a_i a_i^\dagger = 1$, but operators on different sites commute. $J_{ij} = N^{-1}$ for all pairs, and $J_{ii} = \mu + h_i$, where μ is the chemical potential and h_i is a random on-site energy. We recall that [2] in the absence of disorder there are two phases of the model: For generic fillings the bosons can propagate. Thus at zero temperature they form a superfluid. On the other hand, for precisely one boson per site, the particles localize in a Mott insulating phase. When we take away a single particle from this insulator, the resulting hole will behave exactly as the first particle added to the empty lattice. This can be proven by performing a particle-hole transformation on the Hamiltonian.

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In what follows we approach the localized phase from two directions. First, from the Mott insulator by adding holes. In this case a one-particle approach clearly suffices. We calculate the density of states (DOS) and the participation ratio, and show that above a critical disorder the ground state becomes localized. Critical exponents will be evaluated as well. Second, we approach the same phase by decreasing the density of holes from the extended phase and compute the superfluid order parameter and the susceptibility.

In studying the one-particle problem, the quenched disorder averaging $\langle\cdots\rangle_{\text{ave}}$ is performed with the replica trick, allowing us to rewrite the DOS as

$$\rho(\lambda) = \frac{1}{N}\left\langle \sum_k \delta(\lambda + J_k)\right\rangle_{\text{ave}} = \lim_{n\to 0}\frac{2}{N\pi}\,\mathrm{Im}\frac{\partial}{\partial\lambda}\frac{\partial}{\partial n}\int [dx_{i\alpha}]\,d\mathbf{h}\,P(\mathbf{h})e^{-(\lambda/2)\sum_{i\alpha}x_{i\alpha}^2-(1/2)\sum_{ij\alpha}J_{ij}x_{i\alpha}x_{j\alpha}}. \tag{2}$$

λ is an energy eigenvalue with a positive infinitesimal imaginary part, and the J_k's are the eigenvalues of the J matrix. Next the off-diagonal terms are decoupled using an auxiliary field z_α, and the x integrals are performed to transform the exponent into

$$S_{\text{eff}} = -\frac{1}{2}\sum_\alpha z_\alpha^2 + N\ln\left\langle \exp\left[-\frac{n}{2}\ln(\lambda - h) - \frac{1}{2N}\frac{1}{(\lambda - h)}\sum_\alpha z_\alpha^2\right]\right\rangle, \tag{3}$$

where the averaging over the disordered site energies $\int dh\,P(h)A(h)$ is denoted by $\langle A(h)\rangle$. In the expectation value we use the inverse of the number of lattice sites N as a small parameter to carry out an exact expansion. We also keep only the terms linear in the replica number n to arrive at the exponent

$$S_{\text{eff}} = -\frac{1}{2}\left(\left[1 + \left\langle\frac{1}{\lambda - h}\right\rangle\right]\sum_\alpha z_\alpha^2 + Nn\langle\ln(\lambda - h)\rangle\right). \tag{4}$$

Finally performing the integration over the auxiliary field z_α yields

$$\rho(\lambda) = -\frac{1}{\pi}\mathrm{Im}\left\langle\frac{1}{\lambda - h}\right\rangle - \frac{1}{N\pi}\mathrm{Im}\frac{\partial}{\partial\lambda}\ln\left(1 + \left\langle\frac{1}{\lambda - h}\right\rangle\right) = P(\lambda) + \frac{1}{N}\delta(\lambda + \lambda_0), \tag{5}$$

where λ_0 is obtained from $\langle(\lambda_0 - h)^{-1}\rangle = 1$. We assume that $P(h)$, the distribution of the site energies, is nonzero on the interval $(-\Delta, \Delta)$.

The DOS was easiest to obtain in the above path-integral framework, but the subsequent physical quantities can be determined by the simpler method of calculating the eigenvectors $\varphi(\lambda)$ of the J matrix. One finds $\varphi_i(\lambda) = m/(\lambda - h_i)$, where m is the superfluid order parameter: $m = (1/N)\sum\varphi_i$. The self-consistency equation for m yields $1 = (1/N)\sum 1/(\lambda - h_i)$. If λ is inside $P(h)$, then a few $\varphi_i(\lambda)$'s will be $\sim\mathcal{O}(1)$ and the rest of the $\varphi_i(\lambda)$'s will be $\sim\mathcal{O}(1/N)$ to satisfy the normalization condition; i.e., the states inside the continuum are localized, whereas for λ_0 outside the continuum *all* $\varphi_i(\lambda_0) \sim \mathcal{O}(1/\sqrt{N})$, describing an extended state. This picture is in complete accordance with the above-determined DOS. The ground state becomes localized if $-\lambda_0$ reaches the bottom of the band. This does not happen for a rectangular distribution since explicit calculation yields $\lambda_0 = \Delta\coth\Delta > \Delta$. However, for the triangular distribution $P(h) = \Delta^{-2}(\Delta - |h|)$ the ground state eigenvalue $-\lambda_0$ is given implicitly by the equation

$$\Delta^2 = (\lambda_0 - \Delta)\ln\frac{\lambda_0 - \Delta}{\lambda_0} + (\lambda_0 + \Delta)\ln\frac{\lambda_0 + \Delta}{\lambda_0}, \tag{6}$$

which is valid only for $\lambda_0 > \Delta$. Taking the $\lambda_0 \to \Delta + 0$ limit in Eq. (6) shows that $-\lambda_0$ reaches the bottom of the band at the critical disorder $\Delta_c = 2\ln 2 = 1.38$. For $\Delta > \Delta_c$ the DOS becomes identical to the distribution of the site energies, i.e., $\rho(\lambda) = P(\lambda)$.

One measure of localization is the participation ratio $\mathcal{P} = (\sum_i|\varphi_i|^2)^2/(\sum_i|\varphi_i|^4)$. $\mathcal{P}$ is proportional to the system size N for extended states and remains $\sim\mathcal{O}(1)$ for localized ones. The expression for φ_i yields

$$\frac{\mathcal{P}}{N} = \frac{\langle(\lambda_0 - h)^{-2}\rangle^2}{\langle(\lambda_0 - h)^{-4}\rangle}, \tag{7}$$

for $\Delta < \Delta_c$ and $\mathcal{P}/N = 0$ for $\Delta > \Delta_c$. For the uniform distribution there is no critical disorder, and the participation ratio is $\mathcal{P}/N = 3/(3\cosh^2\Delta + \sinh^2\Delta) \sim \mathcal{O}(1)$, clearly indicating that the ground state remains extended for any finite disorder strength. For the triangular distribution the result of the integral (7) is

$$\frac{\mathcal{P}}{N} = \frac{3\lambda_0^2}{3\lambda_0^2 - \Delta^2}\left(\frac{\lambda_0^2 - \Delta^2}{\Delta^2}\right)^2\ln^2\frac{\lambda_0^2 - \Delta^2}{\lambda_0^2}, \tag{8}$$

and λ_0 is obtained from Eq. (6) for $\Delta < \Delta_c$. As λ_0 approaches Δ, $\mathcal{P}/N$ disappears as $\propto(\Delta_c - \Delta)^2$, indicating that for $\Delta > \Delta_c$ the ground state becomes *localized*. From now on we will focus only on this more interesting case of the triangular distribution.

One can independently test these results numerically by diagonalizing the matrix J and measuring $\mathcal{P}$. Figure 1 displays convincing agreement between analytic results (solid line) and numerical results (symbols). The crossing and subsequent decrease of $\mathcal{P}$ with N (inset) provides compelling evidence for the localization of the ground state.

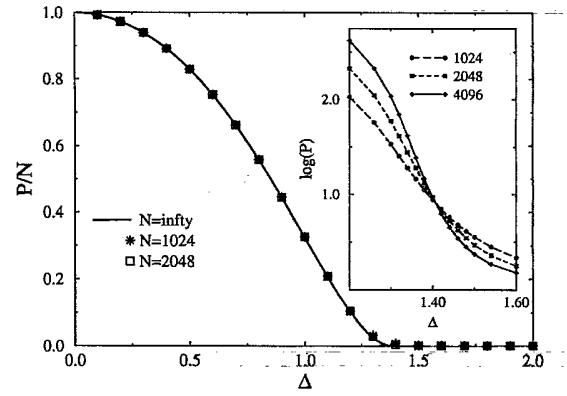

FIG. 1. Analytical and numerical results for the ground state participation ratio.

To demonstrate how $\mathcal{P}$ distingishes between extended and localized states, one usually considers two possibilities, $\varphi_i = 1/\sqrt{N}$ and $\varphi_i = \delta_{i,i_0}$. These yield $\mathcal{P} = N$ and $\mathcal{P} = 1$, respectively. One often equivalently phrases this analysis in terms of the inverse participation ratio $\mathcal{P}^{-1}$, which takes on small values $\mathcal{O}(1/N)$ for extended states and values near unity for localized ones. However, if φ_i has a few large amplitudes on selected sites, and an extended background, $\varphi_i = [1/2]\delta_{i,i_0} + 1/\sqrt{2(N-1)} \times (1 - \delta_{i,i_0})$, $\mathcal{P}$ and $\mathcal{P}^{-1}$ will be close to 1 and indicate, incorrectly, that the state is localized. To eliminate the possibility of misidentifying such "pseudolocalized" states, we computed $\mathcal{P}^{-1}(n)$, which we define by systematically removing the n sites where the wave function assumes its largest values. We show the results of this calculation in Fig. 2.

When $\Delta = 1.0 < \Delta_c$, the ground state is extended, and $\mathcal{P}^{-1}(n)$ remains $\mathcal{O}(1/N)$ as sites are removed. Meanwhile, for all the excited states, $\mathcal{P}^{-1}$ rapidly plunges to much smaller values than $\mathcal{O}(1/N)$, emphasizing that as a few sites are removed from the sum, the weight of the remaining sites is negligible. We checked this behavior on different lattice sizes, and found that $\mathcal{P}^{-1}(n)$ fell slightly *more* rapidly with n for larger lattices, eliminating the possibility that the states were extended but over a small fraction of the lattice. We conclude that all states in the continuum are indeed localized. When $\Delta = 1.7 > \Delta_c$, even the ground state is localized, as shown.

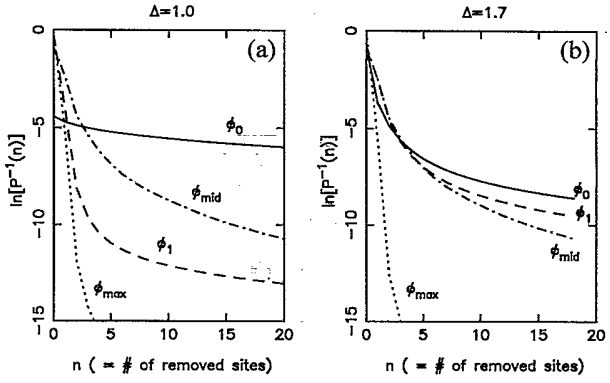

FIG. 2. The truncated participation ratio. Here the four indices refer to the ground state, first excited state, a midband, and the maximal energy wave functions.

Returning to the analytic calculations, the transition can be parametrized by the chemical potential as well. If μ exceeds a critical value μ_c, then the ground state has no holes. At μ_c the first hole appears in the system. μ_c is given by the lowest eigenvalue of the $-J$ matrix, i.e., $\mu_c = \lambda_0$ for $\Delta < \Delta_c$ and $\mu_c = \Delta$ for $\Delta > \Delta_c$. The transition is well captured by the imaginary time on-site Green's function [6]

$$g(\tau) \equiv \frac{1}{N}\sum_i \langle T_\tau a_i^\dagger(\tau) a_i(0)\rangle_0 = \int d\lambda\, \rho(\lambda) \exp[-\tau(\mu - \lambda)], \qquad (9)$$

for $\tau > 0$, where $\langle\cdots\rangle_0$ is the ground state expectation value, and T_τ is the time ordering operator. For weak disorder the transition happens to the state at $-\lambda_0$. Combining Eqs. (5) and (9) one obtains *at criticality* $g(\tau) \approx 1/N + \exp[-\tau(\lambda_0 - \Delta)]$ near the transition, for $\tau \gg 1$. On the other hand, for strong disorder ($\Delta > \Delta_c$) the critical $g(\tau)$ decays as $g(\tau) \propto \tau^{-2}$. This change of the critical behavior suggests that we enter into different phases for $\Delta < \Delta_c$ and $\Delta > \Delta_c$. It is worth noting that if the distribution $P(h) \propto (\Delta - h)^\alpha$, then in the strong disorder regime $g(\tau) \propto \tau^{-\alpha-1}$ right at the critical point. This means that in the strong disorder regime the critical exponent depends on the distribution of the disorder.

If one approaches the same localized phase from higher densities of holes, these one-particle techniques must be abandoned. We will concentrate on the free energy of the Hamiltonian (1), $f = k_B T \ln Z/N$, where $Z = \mathrm{Tr}\exp(-\beta H)$. Introducing the magnetization m as a Hubbard-Stratonovich field decouples the different sites to yield a single site problem,

$$f = \frac{1}{4}m^2 - \frac{1}{\beta N}\sum_i \ln Q_i, \qquad (10)$$

where

$$Q_i = \mathrm{Tr}\exp\beta[(\mu + h_i)a^\dagger a + (ma^\dagger + m^* a)/2]. \qquad (11)$$

For hard-core bosons the Hilbert space is only two dimensional, as a site may be only empty or occupied by one particle. This allows the exact evaluation of Q and hence the free energy per site, which we give here only for $T = 0$,

$$f = \tfrac{1}{4}m^2 - \tfrac{1}{2}\langle(\mu - h) + \sqrt{(\mu - h)^2 + m^2}\rangle. \qquad (12)$$

m is determined by the saddle-point condition, $m = m\langle[(\mu - h)^2 + m^2]^{-1/2}\rangle$. The order parameter m is proportional to $\langle a_i\rangle$. The hard-core boson problem is equivalent to a spin 1/2 XY model in a transverse field, and m corresponds to the magnetization in the XY plane. Long range order is a nontrivial concept on infinite connectivity

lattices. However, if one deduces it from the extensiveness of an eigenvalue of the density matrix [7], the same results pertain.

$m = 0$ is always a solution, but upon exiting the Mott insulator below a critical chemical potential μ_c another solution with nonzero magnetization m appears. For weak disorder $\Delta < \Delta_c$, $\mu_c = \lambda_0$. Expanding in m near the critical point the magnetization behaves the same way as it does without disorder, i.e., $m \propto \sqrt{\mu_c - \mu}$, the well-known Landau result.

In the strong disorder regime when increasing the density, the particles occupy localized states. Do we have a superfluid in this case? In order to get the answer, we write out the saddle-point equation for the triangular distribution,

$$\Delta^2 = \mu_+ \ln\left(\frac{\mu_+ + \sqrt{\mu_+^2 + m^2}}{\mu + \sqrt{\mu^2 + m^2}}\right) + \mu_- \ln\left(\frac{\mu_- + \sqrt{\mu_-^2 + m^2}}{\mu + \sqrt{\mu^2 + m^2}}\right) + 2\sqrt{\mu^2 + m^2} - \sqrt{\mu_+^2 + m^2} - \sqrt{\mu_-^2 + m^2}, \tag{13}$$

where we have introduced the notation $\mu_+ = \mu + \Delta$ and $\mu_- = \mu - \Delta$. For strong disorder $\mu_c = \Delta$, because if μ is slightly below Δ, i.e., μ_- is negative, one sees immediately from the second term of the right-hand side (RHS) of Eq. (13) that m must be different from zero, otherwise the logarithm "blows up." Clearly a superfluid is formed, even though the underlying one-particle states are localized [8].

The above results clearly show that the truly localized phase occupies only a line in the μ-Δ plane. However, we think that this is indeed the seed of the "Bose-glass" phase, because for the finite range hopping model if one partitions the system into blocks of the size of the hopping length, each will support only one of these truly localized, nonsuperfluid states. There will be a macroscopic number of these blocks, thus the original line will expand into a finite region as a function of the density.

The one-particle states being localized, it is natural to assume that $m \ll \mu_c - \mu = |\mu_-|$. In this case the second term of the RHS of Eq. (13) behaves like $\mu_- \ln(m^2/|\mu_-|)$, and this term must be finite, so we find

$$m \propto \sqrt{\mu_c - \mu} \exp\left(-\frac{a}{\mu_c - \mu}\right), \tag{14}$$

where $a = \Delta(\Delta - \Delta_c)/2$. As we can see, below μ_c the system is superfluid, though the magnetization is much smaller than in the weak-disorder case. The critical behavior is again different in the weak and strong disorder regimes. It is remarkable that in the study of the corresponding one-dimensional problem essential singularities were found also [9].

Finally we calculate the susceptibility by adding an infinitesimal in-plane field B to m and taking $\chi = -\partial^2 f/\partial B^2$. Approaching the transition from the $m > 0$ side for arbitrary disorder we get $\chi \propto (\mu - \mu_c)^{-1}$. On the other hand, approaching from the nonsuperfluid side (i.e., $m = 0$), while for weak disorder one again obtains $\chi \propto (\mu - \mu_c)^{-1}$, for strong disorder χ remains finite even *at* the transition. This difference of the exponents again demonstrates that the transitions from the Mott insulator into the superfluid or into the localized region belong to different universality classes, further strengthening the argument that the localized region, in fact, is a separate phase. Just as for the Green's function, the above exponents also depend on the asymptotics of the disorder distribution for strong disorder.

To summarize, we investigated the disordered hard-core boson problem. We proved that, contrary to previous beliefs, a well chosen mean-field theory is capable of capturing the localization transition. We approached the localized region both from the Mott insulator and from the superfluid phase, calculating the density of states, the inverse participation ratio, the on-site Green's function, the magnetization, and the susceptibilty. We tested our theory with independent numerical investigations and found detailed agreement. The key observation is that the exponents of all of the above physical quantities *differ* for the direct insulator-superfluid and the insulator-glass or superfluid-glass transitions, clearly demonstrating that the glass transition belongs to a new universality class. We also gave a real space blocking argument why we expect the glass to expand into a region in the parameter space when the range of hopping is reduced to finite values.

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