Bose-Einstein Condensation in Quantum Glasses

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The role of geometrical frustration in strongly interacting bosonic systems is studied with a combined numerical and analytical approach. We demonstrate the existence of a novel quantum phase featuring both Bose-Einstein condensation and spin-glass behavior. The differences between such a phase and the otherwise insulating "Bose glasses" are elucidated.

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*Introduction.—*Quantum particles moving in a disordered environment exhibit a plethora of nontrivial phenomena. The competition between disorder and quantum fluctuations has been the subject of vast literature [1,2] in past years, with a renewed interest following from the exciting frontiers opened by the experimental research with cold atoms [3,4]. One of the most striking features resulting from the presence of a disordered external potential is the appearance of localized states [1]. Localization happens both for fermions and bosons [2], but in the latter case one has to introduce repulsive interactions to prevent condensation of particles in the lowest energy state. This results in the existence of an insulating phase called "Bose glass," characterized by a finite compressibility and gapless density excitations in sharp contrast to the Mott insulating phase [2,5].

On the other hand, latest research stimulated by the discovery of a supersolid phase of helium has brought to the theoretical foresight of a "superglass" phase [6,7], corroborated by recent experimental evidence [8], where a metastable amorphous solid features both condensation and superfluidity, in the absence of any random external potential. The apparent irreconcilability, between the current picture of insulating "Bose glasses" and the emergence of this novel phase of matter, calls for a moment of thought. Although it has been recently demonstrated that attractively interacting lattice bosons can overcome the localization induced by an external random potential and feature a coexistence of superfluidity and amorphous order [9], a general understanding of the physics of Bose-Einstein condensation in quantum glasses and in the presence of purely repulsive interactions is still in order. In particular, we wonder what could be the possible microscopic mechanism leading to superglassines and if the external disorder, current paradigm in the description of quantum glasses, could be replaced by some other mechanism.

In this Letter we show that geometrical frustration is the missing ingredient. Geometrical frustration is a well recognized feature of disordered phases in which the translational symmetry is not explicitly broken by any external potential. Examples are spin liquids phases of frustrated magnets [10], valence-bond glasses [11], and the order-by-disorder mechanism inducing supersolidity on frustrated lattices [12]. Another prominent manifestation of frustration is the presence of a large number of metastable states that constitutes the fingerprint of spin glasses. When quantum fluctuations and geometrical frustration meet, their interplay raises nontrivial questions on the possible realization of relevant phases of matter. Most pertinently to our purposes: can quantum fluctuations stabilize a superglass phase in a self-disordered environment induced by geometrical frustration? Hereby we answer this question demonstrating that repulsively interacting bosons can feature a low-temperature phase characterized both by spin-glass order and Bose-Einstein condensation. Such a frustration induced superglass sheds light onto a novel mechanism for glass formation in bosonic systems noticeably different from the localization effects leading to "Bose glass" insulators and paving the way to a better understanding of this new phase of the matter.

*Model.—*Strongly interacting bosons on a lattice can be conveniently described by means of the extended Hubbard Hamiltonian, namely

$$\widehat{\mathcal{H}} = -t\sum_{\langle i,j\rangle}[b_i^\dagger b_j + b_i b_j^\dagger] + V\sum_{\langle i,j\rangle} n_i n_j, \tag{1}$$

where $b_i^\dagger(b_i)$ creates (destroys) a hard-core boson on site i, $n_i = b_i^\dagger b_i$ is the site density, and the summations over the indexes $\langle i, j\rangle$ are extended to nearest-neighboring vertices of a given lattice with L sites. In the following, we will set $t = 1$; i.e., we will measure all energies in units of t. In this work, to capture the essential physics of the problem in exam, we adopt a minimal and transparent strategy to induce geometrical frustration in the solid. We therefore consider the set of all possible graphs of L sites, such that each site is connected to exactly $z = 3$ other sites, and we

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give the same probability to each graph in this set. We will discuss average properties over this ensemble of random graphs in the thermodynamic limit $L \to \infty$. The motivations for the choice are the following. (i) On a square lattice, model (1) is known to produce a solid insulating phase at high enough density, where the particles are arranged in a checkerboard pattern [13]. This is due to the fact that all loops have even length. On the contrary, typical random graphs are characterized by loops of even or odd length; in the classical case $t = 0$, this frustrates the solid phase enough to produce a thermodynamically stable glass phase at high density [14]. (ii) Typical random graphs have the important property that they are locally isomorphic to trees, since the size of the loops scales as $\ln L$ for large L: indeed, this is a consistent way of defining Bethe lattices without boundary [14]. The locally treelike structure allows us to solve the model exactly, at least in the liquid phase, by means of the cavity method [15,16]. (iii) These lattices are quite different from square lattices. Yet, it has been shown in the classical case, and for some more complicated interactions, that the phase diagram is qualitatively very similar for the model defined on a random graph and on a square lattice [17,18]. Hence, we believe that it is possible to find a model similar to Eq. (1), defined on a square lattice but with slightly more complicated interactions (probably involving many-body terms) that will show the same qualitative behavior of the model investigated here.

Methods.—The stochastic sampling of the quantum partition function $\mathcal{Z} = \mathrm{Tr} e^{-\beta \hat{\mathcal{H}}}$ at finite temperature $T = 1/\beta$ can be conveniently exploited to obtain numerically exact properties of a generic bosonic Hamiltonian such as (1). Quantum Monte Carlo schemes based on the original worm algorithm idea [19] have been recently extended to canonical ensemble simulations [20,21]. These methods offer an efficient scheme based on the sampling of the configuration space spanned by the extended partition function $\mathcal{Z}_w(\tau) = \mathrm{Tr} e^{-(\beta-\tau)\hat{\mathcal{H}}} \hat{W} e^{-\tau \hat{\mathcal{H}}}$, where $\hat{W}$ is a suitable worm operator determining an imaginary-time discontinuity in the world lines. We have chosen the worm operator introduced in [21], which is a linear superposition of n-body Green functions, avoiding the complications arising in [20] where the commutability of the worm operator with the nondiagonal part of the Hamiltonian is required. Full details of the stochastic Green function (SGF) method are described in Ref. [21]; we only stress here that access to exact equal-time thermal averages of n-body Green functions is granted as well as to thermal averages of imaginary-time correlation functions of local, i.e., diagonal in the occupation numbers representation, quantum operators.

A different and complementary approach to models defined on random lattices consists in solving them exactly in the thermodynamic limit $L \to \infty$, by means of the cavity method [14]. Since local observables are self-averaging in this limit, this results in automatically taking into account the average over the different realizations of the random graphs. For bosonic systems, the cavity method allows us to reduce the solution of the model to the problem of finding the fixed point of a functional equation for the local effective action, in a similar spirit to bosonic dynamical mean field theory. All the details of the computation have been discussed in [16], where it has been shown that the method allows us to compute the average of all the relevant observables. However, in the simplest version discussed in [16], the cavity method can only describe homogeneous pure phases such as the low-density liquid. In order to describe exactly the high density glassy phase, where many different inhomogeneous states coexist, one has to introduce a generalization of the simplest cavity method which goes under the name of replica symmetry breaking (RSB). Unfortunately, this is already a difficult task for classical models, in particular, in spin-glass-like phases [14]. Hence, in this paper we describe the glassy phase using the simplest version of the method, the so-called replica symmetric (RS) one. This yields an approximate description of the glassy phase which we expect to be qualitatively correct. To summarize, in the low-density liquid phase we can compute averages numerically with SGF and analytically with the cavity method, and we obtain a perfect agreement between the two results. In the glassy phase, the RS cavity method is only approximate, an exact solution for $L \to \infty$ requiring the introduction of RSB. On the other hand, SGF is limited for large L by the unavoidable divergence of equilibration times due to the glassy nature of the system. Still, we find a good agreement between the result of SGF for fairly large L, where the system can still be equilibrated, and the RS cavity method for $L \to \infty$, making us confident that the qualitative and quantitative picture of the glassy phase we obtained here is fully consistent. Moreover, we solved the model at the simplest (one-step) RSB level in some selected state points and we found a very small quantitative difference with the RS solution.

Results.—The presence of off diagonal long range order can be conveniently detected by considering the large separation limit of the one-body density matrix; i.e., the condensate reads

$$\rho_c = \lim_{|i-j|\to\infty} \overline{\langle b_i^\dagger b_j \rangle} = \overline{|\langle b_i \rangle^2|}, \tag{2}$$

where the square brackets indicate a quantum and thermal average and the bar indicates averages over independent realizations of the random graphs. The cavity method works in the grand-canonical ensemble and gives direct access to the average of b, while canonical ensemble simulations done with SGF give easy access to the one-body density matrix. On the other hand, spin-glass order is signaled by the breaking of translational invariance, namely $\langle n_i \rangle \neq L^{-1} \sum_{i=1}^{L} \langle n_i \rangle = \rho$. Introducing $\delta n_i = (n_i - \rho)$, the on site deviation from the average density, spin-glass order can be quantified by the Edwards-

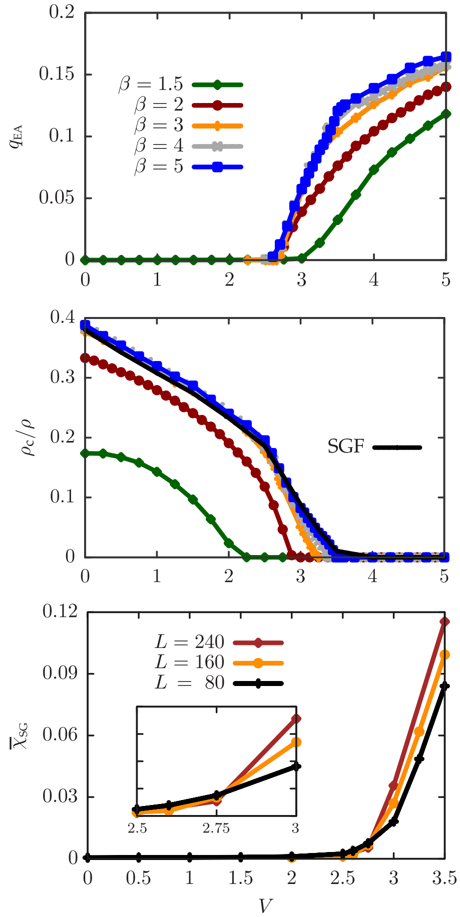

FIG. 1 (color online). Edwards-Anderson order parameter (top) and condensate fraction ρ_c/ρ (middle) as functions of V at half-filling, computed via the cavity method at different values of β. In the middle panel ρ_c/ρ as obtained by SGF at $\beta = 5$ is reported. (Bottom) Scaled spin-glass susceptibility $\bar{\chi}_{SG} = \chi_{SG}/L^{5/6}$ reported as a function of V; standard finite-size-scaling arguments [22] show that the different curves must intersect at the spin-glass transition.

Anderson (EA) order parameter

$$q_{EA} = \frac{1}{L}\sum_{i=1}^{L}\overline{\langle\delta n_i\rangle^2}, \tag{3}$$

which can be easily computed by the cavity method, or by the divergence of the spin-glass (SG) susceptibility

$$\chi_{SG} = \frac{1}{L}\int_0^\beta d\tau \sum_{i,j}\overline{\langle\delta n_i(0)\delta n_j(\tau)\rangle^2}, \tag{4}$$

which is more easily accessible in SGF. It is possible to show [22] that χ_{SG} is the susceptibility naturally associated to the order parameter q_{EA}, because it can be defined as the derivative of q_{EA} with respect to an external field coupled to the order parameter itself (as in standard critical phenomena).

At half-filling factor $\rho = 1/2$, the condensate fraction, the Edwards-Anderson order parameter, and the scaled spin-glass susceptibility are shown in Fig. 1. In the middle panel we compare the values of the condensate fraction obtained via the cavity method and via SGF in a linear extrapolation to $L \to \infty$. The very good coincidence of these results supports our conjecture that the approximate RS description of the glass phase we adopted here is quantitatively and qualitatively accurate. At the lowest temperature, the system becomes a glass around $V \sim 2.7$ while it still displays Bose-Einstein condensation; the condensate fraction only vanishes at $V \sim 3.5$ inside the glass phase. This clearly establishes the existence of a zero-temperature superglass phase in the region $2.7 \lesssim V \lesssim 3.5$. Note additionally that both transitions are of second order; hence, the condensate fraction is a continuous function. Since the latter stays finite on approaching the spin-glass transition from the liquid side (where the cavity method gives the exact solution), it must also be finite on the glass side just after the transition. In Fig. 2 we report the finite temperature phase diagram of the model at half-filling. It is defined by two lines: the first separates the noncondensed ($\langle b\rangle = 0$) from the Bose-Einstein condensation ($\langle b\rangle \neq 0$) phase; the second separates the glassy ($q_{EA} \neq 0$) from the liquid ($q_{EA} = 0$) phase. The intersection between these two lines determines the existence of four different phases (normal liquid, superfluid, normal glass, superglass).

Ground-state degeneracy.—Geometrical frustration induces the existence of a highly degenerate set of ground states, each of them characterized by a different average on-site density, which is absent in glassy phases induced by localization in disordered external potentials such as the Bose glass. To demonstrate this peculiar feature, it is instructive to consider a variational wave function explicitly breaking the translational symmetry of the lattice

$$\langle \mathbf{n}|\Psi_\alpha\rangle \propto \exp\left[\sum_i \alpha_i n_i\right], \tag{5}$$

where the variational parameters α_i are explicitly site dependent and tend to (dis)favor the occupation of a given site. In the spin-glass phase of the bosons, the optimal set of the variational parameters is highly dependent on the

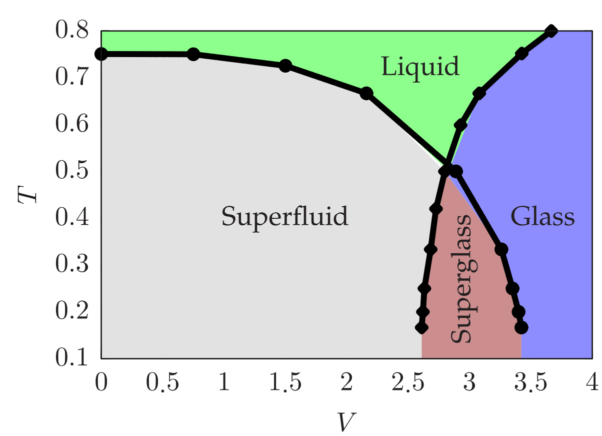

FIG. 2 (color online). Finite temperature phase diagram at half-filling.

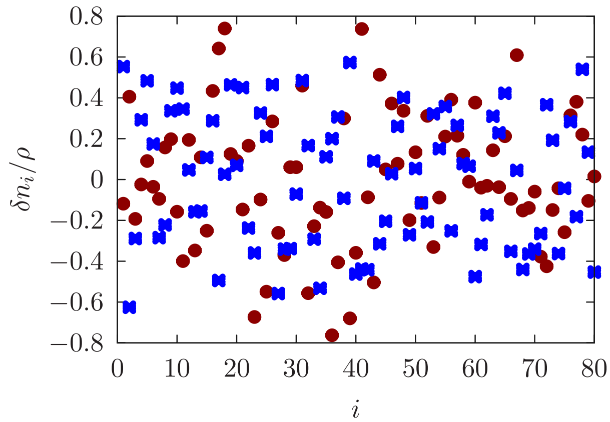

FIG. 3 (color online). Variational expectation values of the site density for different sets of the optimized parameters at half-filling density for $L = 80$ and $V = 4$.

initial conditions associated with the α_i, whereas all the variational states, even with different parameters, have almost degenerate variational energies. Each set of optimized variational parameters is then representative of one of the many degenerate ground states of $\widehat{\mathcal{H}}$. As an example, we show in Fig. 3 the variational expectation values of the site densities for two different solutions resulting from the minimization of the variational energy with the method of Ref. [23], a robust stochastic variant of the Newton method. We further checked, using the zero-temperature Green function Monte Carlo method [24], that if one applies the imaginary-time evolution $|\phi_\alpha\rangle = \exp(-\tau\widehat{\mathcal{H}})|\Psi_\alpha\rangle$ to one of these states, the density profile remains amorphous for a time τ that is divergent with the size of the system.

Conclusions.—The aim of this Letter is to show the existence of a stable superglass phase in a lattice model of geometrically frustrated bosons, in the absence of quenched disorder in the Hamiltonian. This has been done by combining the analytical solution of the model via the quantum cavity method and numerical simulations via quantum Monte Carlo calculations. The glass phase we found is very different from the usual Bose glass, since the latter is driven by localization effects in the presence of an external disorder and is then insulating, while the former is driven by self-induced frustration on a disordered lattice and displays Bose-Einstein condensation. This results in a coexistence of a large number of degenerate amorphous ground states, whose existence we showed by a variational argument corroborated by quantum Monte Carlo calculations. We expect, by analogy with the classical case [17], that the glassy phase found here will exist also on regular finite dimensional lattices, provided the interactions are modified to induce sufficient geometrical frustration. In that case, its properties should be very similar to the one showed by metastable superglasses observed both in numerical simulations [6] and experiments [8] on helium 4. The main difference is that, due to the randomness of the underlying lattice, the superglass studied here is a truly stable equilibrium state, allowing for a much more precise characterization of its properties.

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Note added in proof.—After this work was completed, we became aware of the paper [25] where related results have been obtained.

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