Gaussian Theory of Superfluid—Bose-Glass Phase Transition

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We show that Gaussian quantum fluctuations, even if infinitesimal, are sufficient to destroy the superfluidity of a disordered boson system in 1D and 2D. The critical disorder is thus finite no matter how small the repulsion is between particles. Within the Gaussian approximation, we study the nature of the elementary excitations, including their density of states and mobility edge transition. We give the Gaussian exponent η at criticality in 1D and show that its ratio to η of the pure system is universal.

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In the presence of disorder (repulsive), interacting bosons can undergo a $T = 0$ transition from the superfluid (SF) phase into an insulating Bose-glass (BG) phase [1–8]. The disordered boson system is directly relevant to certain physical systems like ^{4}He in porous media [9] and dirty superconductors [10], and less directly to others like the quantum Hall effect [11]. This transition is intrinsically quantum in nature in that no amount of disorder will destroy the superfluidity without invoking the noncommutativity of density n and phase ϕ. As such, it is representative of quantum phase transitions driven by disorder which does not couple directly to the phase of the order parameter. Hence, the usual saddle point or Hartree solution is always long-range ordered (LRO), and corresponds to a nonuniform condensate. Given that it is of interest to investigate what "minimal" quantum effects are necessary to give a transition. In terms of going beyond the saddle point approximation, these effects can be characterized as Gaussian, nonlinear, topological (as in vortices), etc. In effect, one is asking "what drives the transition," even if the true universality class of the transition may require quantum fluctuations beyond the "minimal" ones. To clarify this perspective, consider the 2D classical XY model as an analogy. There, spin waves alone can explain why the low temperature phase is algebraic, even though (bound) vortices do renormalize the exponent η (universality class). On the other hand, vortices must be invoked to explain the Kosterlitz-Thouless transition.

In this Letter we show that Gaussian fluctuations, even if infinitesimal, are sufficient to destroy superfluidity in 1D and 2D at finite disorder. The model we use is the hard-core boson model with on-site disorder, which is equivalent to the spin-1/2 XY magnet with a transverse random field [1,3,4]. Written in a rotated frame for later convenience, the Hamiltonian is [5]

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (S_i^z S_j^z + S_i^x S_j^x) - \sum_j h_j S_j^y \ , \qquad (1)$$

where the random field $\{h_j\}$ is given by an independent Gaussian distribution function $P(h_j)$ with width h. We pick this model because while it contains the features believed to be essential for the SF-BG transition, it has a simple classical solution and a "builtin" parameter to systematically investigate quantum fluctuations. It is also of interest as a disordered quantum spin system [3–5].

The off-diagonal LRO of the boson system is related to the magnetic LRO in the x-z plane. The classical solution for this model corresponds to treating the spins as classical vectors. In terms of the bosons, one is dealing with variational wave function of the form $\prod_j (u_j + v_j b_j^\dagger)|0\rangle$, or, equivalently, Jastrow wave functions given by Gutzwiller projection of condensate wave function $(\sum_j \frac{v_j}{u_j} b_j^\dagger)^N |0\rangle$. In Ref. [1], it was shown that while the classical ground state always has LRO, this is not the case when the quantum (specifically $S = 1/2$) nature of the spin operators is taken into account. Following the motivation discussed in the previous paragraph, it is thus of interest to investigate if the destruction of LRO can be achieved by Gaussian quantal effects. This can be studied by means of a spin-wave analysis [5].

Within such an approach, the first question is what would be the signature of destruction of the LRO [12]. Since the spin-wave analysis is an expansion about the ordered state, this destruction is indicated by an instability. Possible scenarios are (1) a diverging fluctuation in the order parameter, (2) negative excitation energies, or (3) complex excitation energies. In the pure case, scenario (1) is observed in 1D. Exact solution for $S = 1/2$ [13] and general understanding of 1D spin systems indicates that these diverging fluctuations destabilize the LRO and the ground state has algebraically decaying correlation functions.

We now derive the spin-wave Hamiltonian [5]. First we generalize Hamiltonian (1) to arbitrary spin S by rescaling $J \to J/S^2$ and $h_j \to h_j/S$. In the infinite S limit, the spins behave classically. Taking the z axis as the ordering axis, the spin on site j lies on the y-z plane at angle

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θ_j from the z axis. Minimizing energy, one finds that all $\cos\theta_j \neq 0$, hence there is LRO, no matter the value of h [1,14]. Defining Holstein-Primakoff bosons with respect to the local (classical) spin orientation, to order $1/S$, one arrives at the quadratic Hamiltonian [5]:

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}\cos\theta_i\cos\theta_j - \sum_j h_j \sin\theta_j - \frac{1}{2S}\sum_{\langle i,j\rangle}\left(J_{ij}a_i^\dagger a_j + K_{ij}a_i a_j + \text{H.c.}\right) + \mathcal{O}\left(\frac{1}{S^{3/2}}\right) , \tag{2}$$

where $J_{ij} = J(1+\sin\theta_i\sin\theta_j) + \frac{h_j}{\sin\theta_j}\delta_{ij}$ and $K_{ij} = J(1-\sin\theta_i\sin\theta_j)$. Equation (2) describes Gaussian fluctuations of strength $1/S$ about the classical ground state. In Ref. [5], Eq. (2) is studied perturbatively for weak disorder. In this paper, we will diagonalize (2) numerically on finite-sized lattices, and will not limit ourselves to weak randomness. This will enable us to study the destruction of LRO. Equation (2) is formally diagonalized by a Bogoliubov transformation $a_j = \sum_\alpha(u_{j\alpha}\gamma_\alpha + v_{j\alpha}\gamma_\alpha^\dagger)$, where α is the eigenstate index. We have taken the u's and v's to be real. The γ's are boson operators if

$$\sum_j(u_{j\alpha}u_{j\alpha'} - v_{j\alpha}v_{j\alpha'}) = \delta_{\alpha\alpha'} , \tag{3}$$

and we seek the solution $\mathcal{H}_{\text{SW}} = E^0 + \sum_\alpha \omega_\alpha\gamma_\alpha^\dagger\gamma_\alpha$, which implies the Bogoliubov equations for u's and v's,

$$\omega u_{j\alpha} = -\sum_{\langle j'\rangle}(J_{jj'}u_{j'\alpha} + K_{jj'}v_{j'\alpha}) ,$$
$$\omega v_{j\alpha} = \sum_{\langle j'\rangle}(K_{jj'}u_{j'\alpha} + J_{jj'}v_{j'\alpha}) , \tag{4}$$

to be "normalized" by the condition (3). For N sites, there are $2N$ eigenstates. For a given solution with eigenvalue ω, there is the complementary solution $u \leftrightarrow v$, with eigenvalue $-\omega$. However, only one of these is consistent with (3), and the other is unphysical, leaving us with N physical solutions. The Goldstone mode, corresponding to uniform spin rotation about the y axis in (1), is given by $u_i = v_i \propto \cos\theta_i$.

We investigate LRO instability in 1D and 2D. Calculations in 1D are done on lattices of size 50–120, averaging over 500 configurations for each value of $\Delta \equiv J/h$, and in 2D on 6×6 to 11×11 lattices averaging over 200 configurations. Note that Δ small implies strong disorder. Instability criteria (2) and (3) are not observed, leaving (1), a diverging fluctuation in the order parameter as the sole possibility. Within the spin wave approximation as formulated, the relevant quantity is

$$\delta m = \frac{1}{N}\sum_j \cos\theta_j \delta\langle S_j^z\rangle = \frac{1}{N}\sum_j\sum_{\alpha\neq 0}\cos\theta_j v_{j\alpha}^2 = \int d\omega\rho(\omega)v^2(\omega) , \tag{5}$$

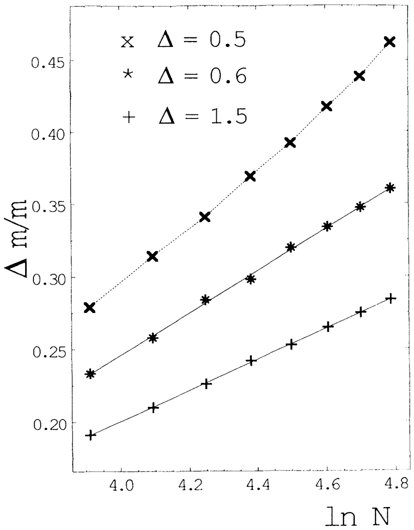

FIG. 1. Fluctuation corrections to the order parameter $\delta m/m$ is plotted against $\ln N$. The divergence becomes faster than $\ln N$ for Δ less than a critical value $\Delta_c \approx 0.6$. The solid lines are obtained through a linear fit and the dashed line is a guide to the eye.

where $\rho(\omega) = \frac{1}{N}\sum_\alpha \delta(\omega - \omega_\alpha)$ is the density of states (DOS).

As remarked earlier, in 1D δm diverges as $N \to \infty$ even without disorder, so it seems criterion (1) is inapplicable. However, more precisely, $\delta m \propto \ln N$, and we view this as an indication for an algebraic LRO (see later), hence the ground state is still a superfluid. Thus, we argue that the transition is marked by δm diverging faster than $\ln N$. This is in fact seen in our calculation, and is shown in Fig. 1, with the critical value of $\Delta = \Delta_c \approx 0.6$, independent of S. The transition occurs thus at finite disorder. Since the spin-wave approximation is correct in the large S limit, there is a discontinuity between $S \to \infty$ and $S = \infty$. In 2D, $\delta m/m$ is finite in the pure case as $N \to \infty$, which we take to mean the LRO is stable, and is consistent with the exact result for $S = 1/2$ [15]. Figure 2 shows $\delta m/m$ vs ln$N$ for different values of Δ, and we see a transition occurring between 0.1 and 0.08.

Thus, in contrast to the classical case, already in the Gaussian approximation a transition to a disordered phase occurs with sufficient disorder. Since in a Gaussian theory the ground state is just the classical state modified by the zero point motion of the excitations, it is of interest to ask whether the transition is due to a change in the DOS $[\rho(\omega)]$ or the nature of the excitations $[v^2(\omega)]$ or both. In the pure case, $v^2(\omega) \propto \frac{1}{\omega}$ and $\rho(\omega) \propto \omega^{d-1}$ for small ω. For the infinitely strong disorder ($J = 0$) case, the excitations are single spin flips, with excitation energies $|h_j|$. It seems reasonable to expect therefore $\rho_0 = \rho(\omega \to 0)$ is finite in 1D for all Δ, and the transition must be due to $v^2(\omega)$ diverging faster than $1/\omega$. This picture is confirmed by our numerical

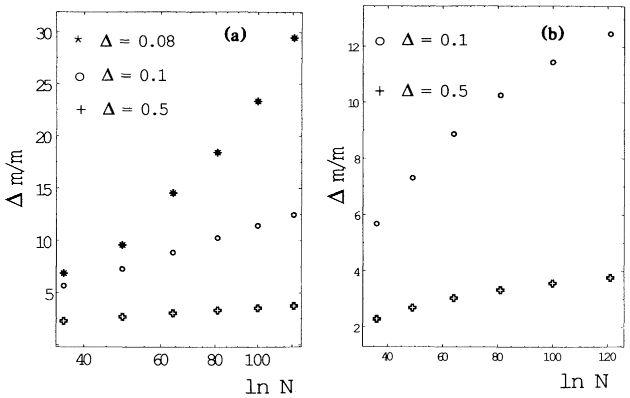

FIG. 2. The same as Fig. 1, plotted for 2D systems. Unlike in 1D, δm is finite for weak disorder and diverges for $\Delta < \Delta_c$, which is between 0.1 and 0.08. (b) The same plot as in (a), but presented on a different scale, which shows clearly that δm is bounded as $N \to \infty$ for large Δ.

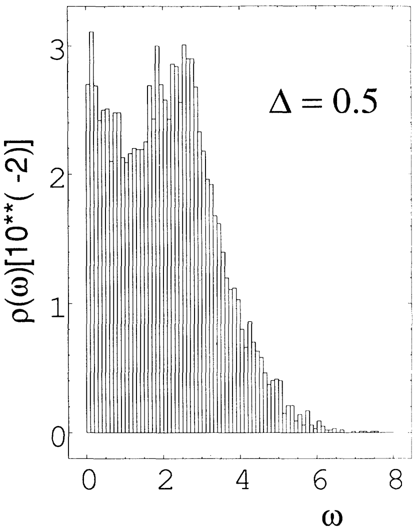

FIG. 3. DOS on the insulating side ($\Delta = 0.5$) in 1D. Here $N = 100$.

calculations (see Fig. 3). The ambiguity in deciding ρ_0 for infinite system from finite-size calculation is reduced by checking the scaling of ρ_0 with N. For $\Delta < \Delta_c$, we find $\delta m \propto N^\theta$, with $\theta = \theta(\Delta)$; while $v^2(\omega) \propto \frac{1}{\omega^\delta}$, with $\delta = 1 + \theta$, again indicating ρ_0 finite. In 2D, the ordered phase should be characterized by $\rho(\omega) \propto \omega$ and the disordered phase by ρ_0 finite. Our results are consistent with this. For $\omega \geq 0.1$, $\rho(\omega)$ is linear in ω, with the slope increasing with decreasing Δ. For $\Delta \leq 0.08$, ρ_0 is finite. The specific heat should thus be $\propto T$ and $\propto T^d$ deep inside the BG and SF phases, respectively. Unfortunately, we cannot say for certain whether the DOS transition exactly occurs at the order parameter transition due to the inability of pinpointing Δ_c. (The popular finite-size scaling method for locating critical point is not applicable here since there is no scale invariance.)

In the SF phase, the low-energy excitations calculated here are approximate solutions of the collective modes (phonons). It is of interest to ask if their localization transition is related to the "localization" of the ground state, or just as an Anderson localization problem. Since the Goldstone mode is always extended, one expects for a given Δ, a transition from extended to localized states with increasing energy at a mobility edge energy E_c. Does $E_c \to 0$ as $\Delta \to \Delta_{c+}$? The quantity we calculate as a measure of localization is the inverse participation ratio p, which we assume for localized states scale as the inverse localization length ξ^{-1}, and is zero for extended states in infinite systems. E_c is the energy below which p vanishes. However, for finite size, p scales as the greater of ξ^{-1}, L^{-1}. Hence, at low energy, where $\xi > L$, $p(E)$ is constant, and only for $E > E_c(L)$, where $p(E_c(L)) = L^{-1}$, does $p(E)$ give the behavior of an infinite system. One way to obtain E_c is by extrapolating that part of the curve to where $p = 0$. An improved method is to extrapolate $E_c(L)$ to $L \to \infty$ [16]. Equation (4) guarantees that $u_{j\alpha}$ and $v_{j\alpha}$ are both either extended or localized, so it suffices to calculate $p(E)$ for $u_{j\alpha}$. In Fig. 4 we show $p(E)$ for various L's in 1D for $\Delta = 1.5$ (SF side) and $\Delta = 0.5$ (insulating side). The former seems to show clearly a finite E_c, while for the latter, we ascertain E_c to be very small, probably zero (our extrapolation actually gives a small unphysical negative value). Within our accuracy of E_c and Δ_c, we determine that $E_c \to 0$ close to, if not at, Δ_c. This seems to support the idea that the localization of the ground state and the excitations occur simultaneously [17].

Upon reflection, however, we have serious doubts. In the perturbative (in disorder) calculation of Ref. [5], the

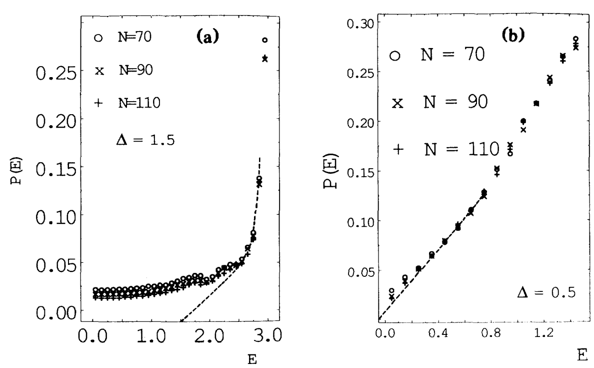

FIG. 4. Participation ratio $p(E)$ in 1D is plotted for several values of N. The pseudomobility edge E_c is obtained from these plots through the procedure described in the main text. In (a), $\Delta = 1.5$, the system is in the superfluid phase and E_c is finite. E_c is zero in the insulating phase as is shown in (b) for $\Delta = 0.5$. The dashed lines are smooth extrapolations to large N.

phonon mean free path is found to diverge as $E^{-(d+1)}$. Common wisdom has it that in 1D, the localization length and the mean free path are essentially identical, since any scattering is backscattering. Hence, one expects the relatively slow $\xi^{-1}(E) \propto E^2$ for small E, crossing over to a more rapid E dependence at a higher energy E_x. This is in fact known to be the case for classical vibrational modes in 1D [18], and all states except the uniform translation mode are localized. The divergence of the localization length ξ is thus not a true critical phenomenon. In our calculation, if the size $L < \xi(E_x)$, then we cannot probe the weak E dependent regime, and we will mistake E_x for the true mobility edge. For comparison, we look at a finite system of random masses connected by springs and find $p(E)$ curves similar to Fig. 4. While our results do not constitute evidence for all eigenstates of (2) to be localized in 1D, we believe this is in fact the case, and what Fig. 4 shows is E_x decreasing as the disorder is increased, vanishing at or close to the SF-BG transition. Since even in 2D it is believed that all classical waves are localized [19], it seems probable that all phonon excitations are localized too. This can be tested experimentally on ^{4}He absorbed on a disordered substrate.

In our model, the classical state is the Gutzwiller state, and $1/S$ serves as an expansion parameter for quantum fluctuations. Since the physics is sufficiently general, we believe the above results would hold true if one considers soft-core (e.g., Hubbard U) models and uses $\hbar$ as the quantum expansion parameter. What about a phase diagram of disorder vs U? Since bosons will condense into the lowest energy (localized) state for $U = 0$, the critical disorder is 0. How about $U \to 0$? The complication is that increasing U both affects the classical condensate and enhances quantum fluctuations. However, provided the product Un remains finite, the Hartree solution is extended even for infinitesimal U [20]. Thus, the $U \to 0$ limit should not be qualitatively different from the limit of $1/S \to 0$. For example, the critical disorder is finite. This conclusion is in agreement with numerical works performed on the disordered boson Hubbard model [8]. Since conventional LRO is stable for weak disorder in 2D, except for trivial dependence on dimensionality, and presumably a finite mobility edge energy for the phonons at weak disorder, the results for 2D should hold for 3D also.

In 1D, based on a perturbative renormalization group calculation, Ref. [17] predicted that the renormalized critical exponent η is universal and equal to 1/3 at the SF-BG transition. One might ask what the value of η is in the Gaussian theory. Rigorously, the spin-wave theory as formulated cannot produce a power-decaying correlation function. [It is similar to using $(\nabla\pi)^2$ as the action in the classical nonlinear σ model.] However, η and γ, the coefficient of $\ln N$ in $\delta m/m$, are proportional in the pure case. Assuming the relation holds even with disorder, it implies $\eta_c/\eta_{\rm pure} = \gamma_c/\gamma_{\rm pure}$. From the slope of the $\Delta = 0.6$ curve in Fig. 1, we estimate $\eta_c/\eta_{\rm pure} \approx 1.4$. This ratio is universal, while η_c is not. $\eta_c \to 0$ as $1/S \to 0$ in our model, or as $U \to 0$ in Hubbard type models.

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