A Gaussian Theory of Superfluid–Bose-Glass Phase Transition

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Abstract

We show that gaussian quantum fluctuations, even if infinitesimal, are suf-
ficient 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 $\eta$ at criticality in 1D and
show that its ratio to $\eta$ of the pure system is universal.

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In the presence of disorder, (repulsive) interacting bosons can undergo a transition from the superfluid (SF) phase into an insulating Bose-glass (BG) phase [1] - [8]. This transition is intrinsically quantum in nature in that no amount of disorder will destroy the superfluidity without invoking the non-commutativity of density $\rho$ and phase $\phi$. Hence, the usual saddle point or Hartree solution is always long-range ordered, and corresponds to a non-uniform 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, non-linear, 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, the true long range order (LRO) is destroyed at any finite temperature by spin waves, even though (bound) vortices do renormalize the exponent $\eta$ (universality class). That is, spin wave alone can explain why the low temperature phase has algebraically decaying correlations. On the other hand, vortices must be invoked to explain the Kosterlitz-Thouless transition [9].

In this article 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]:

$$H = -J \sum_{<i,j>} (S_i^x S_j^x + S_i^y S_j^y) - \sum_j h_j S_j^y,$$

where the random field $\{h_j\}$ is given by 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 ‘built-in’ parameter to systematically investigate quantum fluctuations. It is also of interest as a disordered quantum spin system [3] - [5]. Our study reported in this paper will be focused on the $T = 0$ case.
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 wavefunction of the form $\prod_j (u_j + v_j b_j^+)|0\rangle$, which when projected into states of definite $N$ are Jastrow wavefunctions given by Gutzwiller projection of condensate wavefunction $(\sum_j \frac{u_j}{v_j} b_j^+)^N|0\rangle$. In Ref. [1], it was shown in the spin model that provided there is no gap in the spectrum, the classical ground state is always ordered. However, it was also seen that the ground state is not long range ordered with strong disorder when the quantum (specifically $S = 1/2$) nature of the spin operators is taking 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 [10]. 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 (e.g., Bogoliubov’s solution to bosons with attractive interactions). In the pure case, scenario 1) is observed in 1D. Exact solution for $S = 1/2$ [11] and general understanding of 1D spin systems indicates that this 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 $J \rightarrow J/S^2$ and $h_j \rightarrow h_j/S$. 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 $\theta_j$ from the $z$-axis, with $\{\theta_j\}$ given self-consistently by

$$\sin \theta_j J \sum_{<j'>} \cos \theta_{j'} = h_j \cos \theta_j ,$$

(2)

where $<j'>$ indicates nearest neighbors of the site $j$. The statement that LRO persists to all order is revealed by the solution to (2) having all $\cos \theta_j \neq 0$ no matter what value of $h$ is. A local rotation about the $x$-axis is performed so that the spin points along the new $z$-axis.
The usual Holstein-Primakoff transformation \cite{12} of the spins into b boson operators can now be defined in the rotated frame. To order $1/S$, one arrives at a quadratic Hamiltonian for the bosons \cite{5}:

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

(3)

where $J_{ij} = J(1 + \sin \theta_i \sin \theta_j) + \frac{h_j}{\sin \theta_j} \delta_{ij}$ and $K_{ij} = J(1 - \sin \theta_i \sin \theta_j)$, which describes gaussian fluctuations of strength $1/S$ about the classical ground state. In Ref. \cite{5}, (3) is studied perturbatively for weak disorder. In this paper, we will diagonalize (3) numerically on finite-sized lattices, and will not limit ourselves to weak disorder. This will enable us to study the destruction of LRO. (3) is formally diagonalized by a Bogoliubov transformation \cite{13}:

$$
a_j = \sum_\alpha (u_j a_\alpha + v_j a_\alpha^\dagger),
$$

(4)

where $\alpha$ is the eigenstate index. We have taken the $u$’s and $v$’s to be real. The $\gamma$’s are boson operators if

$$
\sum_j (u_{ja} u_{ja'} - v_{ja} v_{ja'}) = \delta_{aa'},
$$

(5)

and we seek the solution

$$
H_{SW} = E^0 + \sum_\alpha \omega_\alpha \gamma_\alpha^\dagger \gamma_\alpha,
$$

(6)

which implies the Bogoliubov equations for $u$’s and $v$’s,

$$
\omega u_{ja} = -\sum_{<j'>} (J_{jj'} u_{ja'} + K_{jj'} v_{ja'}),
$$

$$
\omega v_{ja} = \sum_{<j'>} (K_{jj'} u_{ja'} + J_{jj'} v_{ja'}),
$$

(7)

to be ‘normalized’ by the condition (5). For $N$ sites, this is a $2N \times 2N$ matrix equations with $2N$ eigenstates. Note that for a given solution with eigenvalue $\omega$, there is the complimentary solution $u \leftrightarrow v$, with eigenvalue $-\omega$. However, only one of these can be consistent with (6),
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 \( 6 \times 6 \) to \( 11 \times 11 \) lattices averaging over 200 configurations. 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

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

(8)

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

As remarked earlier, in 1D \( \delta m \) diverges as \( N \to \infty \) even without disorder, so it seems criteria 1) is inapplicable. However, more precisely, \( \delta m \propto \ln N \), and we view this as an indication for an algebraic LRO (replacing the true LRO, see later), hence the ground state is still a superfluid. Thus, we argue that the transition is marked by \( \delta m \) diverging faster than \( \ln N \). This is in fact seen in our calculation, and is shown in Fig. 1, with the critical value of \( \Delta = \Delta_c \approx 0.6 \) in the present model. 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 \( S = 1/2 \) \[ \text{[14]} \]. Fig. 2 shows \( \delta m/m \) vs. \( \ln N \) for different values, and we see that there is a transition between \( \Delta = 0.1 \) and \( \Delta = 0.08 \).

Thus, already in the gaussian approximation, in contrast to the classical case, there is a transition from an algebraic in 1D and a true long range ordered in 2D superfluid phase to a disordered phase. Since in a gaussian theory, the ground state is just the classical state modified by the zero point motion of the the excitations, it is of interest to ask whether the transition is due to a change in the DOS \( N(\omega) \) or the nature of the excitations \( (v^2(\omega)) \) or both. In the pure case, \( v^2(\omega) \propto \frac{1}{\omega} \) for small \( \omega \), while \( N(\omega) \propto \omega^{d-1} \) for small \( \omega \). For the infinitely strong disorder \( (J = 0) \) case, the excitations are single spin flips, with excitation
energies $|h_j|$. Hence $N(\omega)$ is simply given by the distribution of $h_j$, and is finite at low energies. It seems reasonable to expect therefore $N_0 = N(\omega \to 0)$ is finite in 1D for all $\Delta$, and the transition must be due to $v^2(\omega)$ diverging faster than $1/\omega$. This picture is confirmed by our numerical calculations and Fig. 3 is shown for DOS in 1D. While there is some ambiguity in deciding $N_0$ for infinite system from finite-size calculation, we have checked to see that the scaling of $N_0$ with $N$ is in fact consistent with a non-zero DOS at zero energy. For $\Delta < \Delta_c$, $\delta m \propto N^{\theta}$, with $\theta = \theta(\Delta)$. We find that this exponent is in agreement with the exponent of $v^2(\omega) \propto \frac{1}{\omega^\delta}$, with $\delta = 1 + \theta$, again indicating $N_0$ finite. In 2D, the ordered phase should be characterized by $N(\omega) \propto \omega$ and the disordered phase by $N_0$ finite. Our results are consistent with this. For $\omega \geq 0.1$, $N(\omega)$ is linear in $\omega$, with the slope increasing with decreasing $\Delta$. For $\Delta \leq 0.08$, $N_0$ is finite. Unfortunately, we cannot say for certain whether the DOS transition exactly occurs at the order parameter transition due to the inability of pinpointing $\Delta_c$ (The popular finite-size scaling method for locating critical point is not applicable here since there is no scale invariance). We hope to clear up this point in a later publication.

The low-energy excitations calculated here are particularly significant in the SF phase, as they are approximations to the collective modes (phonons). These excitations can be extended or localized. It is of interest to ask if their localization transition is related to the ‘localization’ of the ground state. It is also of interest by itself as an Anderson localization problem of the eigenstates of (3). Since the zero-mode corresponds to uniform phase rotation, it must be extended. One thus expects that possibly for a given $\Delta$, a transition from extended to localized states with increasing energy at a mobility edge energy $E_c$, and perhaps $E_c \to 0$ 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 $\xi^{-1}$, and is zero for extended states in infinite systems. $E_c$ is the energy where $p$ first vanishes. However, for finite size, $p$ scales as the greater of $\xi^{-1}, L^{-1}$. 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 $p(E)$ gives the behavior of an infinite system. One way to obtain $E_c$ is by extrapolating the part
of the curve to where \( p = 0 \). An improved method is to extrapolate \( E_c(L) \) to \( L \to \infty \) [15].

Eq. (6) guarantees that \( u_{j\alpha} \) and \( v_{j\alpha} \) are either both 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), which for the former seems to show clearly a finite \( E_c \). For the latter, we ascertain \( E_c \) to be very small, probably zero (our extrapolation actually gives an unphysical small negative value). This seems to support the idea that the localization of the ground state and the excitations occur simultaneously, a feature of Giamarchi and Schulz’s theory in 1D [16].

Upon reflection, however, we have serious doubts. In the perturbative (in disorder) calculation of Ref. [5], the 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 cross-over energy \( E_x \). This is in fact known to be the case for classical vibrational modes in 1D [17], and all states except the uniform translation mode are localized. The problem is then that the divergence of the localization length \( \xi \) is not a true critical phenomena with a critical exponent. 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 (3) 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 superfluid-insulator transition. Since even in 2D, it is believed that all classical waves are localized [18], it seems probable that all phonon excitations are localized too. This fact of localization of all the excitations, if it is true, may invalidate the usual effective field theory based on the action of propagating phase modes, which is crucial for the scaling theory of Ref. [2]. Indeed, certain predictions of the scaling theory has been questioned by recent quantum Monte Carlo simulations [19] on 2D hard-core dirty bosons.
In our model, the classical state is the Gutzwiller state, and $1/S$ serves as an expansion parameter for quantum fluctuations. We find a transition at finite disorder when only gaussian fluctuations are kept. Since the physics is sufficiently general, we believe this conclusion would hold true if one consider soft-core (e.g., Hubbard $U$) models and use $\hbar$ 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 = 0. How about $U \to 0$? The problem is that increasing $U$ both affects the classical condensate and enhances quantum fluctuations. In fact, the Hartree solution becomes extended with infinitesimal $U$. Thus, the $U \to 0$ limit should not be qualitatively different from the limit of $1/S \to 0$, and the critical disorder is again finite. This conclusion is in agreement with numerical works performed on the disordered boson Hubbard model [8].

In 1D, Ref. [16] predicted that the renormalized critical exponent $\eta$ is universal and equal to $1/3$ at the SF-BG transition based on a perturbative renormalization group calculation. One might ask what the value of $\eta$ 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 non-linear $\sigma$ model ). However, $\eta$ and $\gamma$, the coefficient of $\ln N$ in $\delta m/m$, are proportional in the pure case. Assuming the relation holds even with disorder, it implies

$$\frac{\eta_c}{\eta_{\text{pure}}} = \frac{\gamma_c}{\gamma_{\text{pure}}}.$$  (9)

From the slope of the $\Delta = 0.6$ curve in Fig. 1, we estimate $\eta_c/\eta_{\text{pure}} \approx 1.4$. This ratio is universal, while $\eta_c$ 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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FIGURES

FIG. 1. Fluctuation corrections to the order parameter $\delta m/m$ is plotted against $\ln N$. The divergence becomes faster than $\ln N$ as $\Delta$ exceeds 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 eyes.

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

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

FIG. 4. Participation ratio $p(E)$ in 1D is plotted for several values of $N$. The pseudo-mobility 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 about zero in the insulating phase as it shows in (b) for $\Delta = 0.5$. 