Probing correlated phases of bosons in optical lattices via trap squeezing

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Abstract. We theoretically analyze the response properties of ultracold bosons in optical lattices to the static variation of the trapping potential. We show that, upon an increase of such a potential (trap squeezing), the density variations in a central region, with linear size of \( \lesssim 10 \) wavelengths, reflect that of the bulk system upon changing the chemical potential: hence measuring the density variations gives direct access to the bulk compressibility. When combined with standard time-of-flight measurements, this approach has the potential of unambiguously detecting the appearance of the most fundamental phases realized by bosons in optical lattices, with or without further external potentials: superfluid, Mott insulator, band insulator and Bose glass.

Ultracold gases in optical lattices offer the unique opportunity of literally implementing fundamental lattice models of strongly correlated quantum many-body systems, either bosonic or fermionic, traditionally considered as ‘toy’ models for the description of complex condensed matter systems [1, 2]. In the particular case of ultracold bosons realizing the Bose–Hubbard (BH) model, recent experimental developments have led to the spectacular demonstration of the Mott insulating (MI) phase with controllable filling [3]–[5], and even more recent developments in laser trapping offer the possibility of realizing further fundamental insulating phases, such as a band insulator (BI) in a commensurate superlattice [6, 7] or a Bose glass (BG) in an incommensurate superlattice or in a laser-speckle potential [8]–[12].

Two main technical aspects limit to date the possibility of the experiments to retrieve full information on the true bulk behavior of the model Hamiltonian implemented in the system.
One aspect is the presence of a parabolic trapping potential which imposes a spatial variation of the filling and hence a spatial modulation of the local behavior exhibited by the system. A second aspect is represented by the typical measurements performed on the system. The detection of strongly correlated phases is typically based on the measurement of correlation functions (phase correlations via time-of-flight measurements [3] and density correlations via noise-correlation analysis [13]) and on siteoccupation statistics [5, 14]. Lattice-modulation spectroscopy offers the possibility of measuring the dynamic structure factor at zero transferred quasi-momentum [12, 15] but it has the drawback of probing the global response of the inhomogeneous system, and of being subject to a low-energy cutoff imposed by the duration of the experiment. This aspect prevents, e.g., the unambiguous observation of the BG, which does not have a special signature in correlation functions, but it is unambiguously marked by the absence of a gap in the excitation spectrum.

The purpose of this paper is to propose a technique—trap-squeezing spectroscopy—which circumvents these two limitations at once, taking advantage of the parabolic trapping to extract the bulk behavior of the model implemented in the system and in particular its lowest particle (hole) excitation energy. Two fundamental observations are at the basis of this proposal. On the one hand, the slowly varying nature of the parabolic potential guarantees the validity of the local-density approximation (LDA) [16]–[19], particularly close to the potential minimum. Hence the density around the trap center mimics the behavior of the bulk system over an extended region of space of linear size of several (\( \gtrsim 10 \)) lattice spacings, and consequently the average density in this region can be accessed via optical microscopy [20]–[22]. On the other hand, this central average density can be controlled via the trapping potential in very much the same way as the chemical potential controls the density of a bulk system in the grand-canonical ensemble. In particular, the trapping potential is by far the lowest-energy potential to which the system is coupled (with trapping frequencies as low as \( \sim 10 \) Hz), and measuring the response of the central density to small variations of such potential allows to directly probe the low-energy response of the bulk system.

We theoretically investigate the trap-squeezing spectroscopy in the one-dimensional (1d) BH model in a parabolic potential plus an external superlattice potential, \( \mathcal{H}(J, U, V_2) + V_1 \sum_i (i - i_0)^2 n_i \), where

\[
\mathcal{H}_0 = \sum_i \left[ -J (b_i^\dagger b_{i+1} + \text{h.c.}) + \frac{U}{2} n_i (n_i - 1) + V_2 g_i n_i \right].
\]

Here \( g_i = g_i(\alpha, \phi) = \cos^2(2\pi \alpha i + \phi) - 1/2 \) is a one-color superlattice potential. \( J \) and \( U \) are experimentally controlled via the height of the primary optical lattice, while \( V_2 \) is controlled via the height of a secondary optical lattice [6, 7, 12]. In the following, we make the fundamental assumption that \( V_i \) can be varied independently of the other parameters, which is possible by applying an extra dipolar trap to the system.

We study the above model via stochastic series expansion quantum Monte Carlo [25] at low temperatures (capturing the \( T = 0 \) behavior) and in the grand-canonical ensemble, namely we simulate the Hamiltonian \( \mathcal{H}_\mu = \mathcal{H} - \mu \sum_i n_i \) where the chemical potential \( \mu \) is fine tuned to get the desired average number of particles \( \langle N \rangle \), and in this way it becomes a function of the other Hamiltonian parameters \( \mu = \mu(V_i, N, J, U, V_2) \). According to LDA, the average density at the center of the trap \( n_C = 1/|C| \sum_{i \in C} n_i \) (where the region \( C \) will be defined later) reproduces closely that of a homogeneous system \( \langle N \rangle = 0 \) at a chemical potential \( \mu \). Hence controlling \( \mu \) via one of the other parameters \( V_i, N, J, U \) and \( V_2 \), allows control of \( n_C \). In particular, if \( \mu \) is
controlled by changing $V_t$, namely by trap squeezing, while holding all the other parameters fixed, one has access to the compressibility for the bulk Hamiltonian $H_0(J, U, V_2)$, estimated via $\kappa = \partial n_C / \partial \mu$.

The control on the chemical potential $\mu$ via trap squeezing requires detailed knowledge of the function $\mu = \mu(V_t, N, J, U, V_2)$. Such a function can be accurately sampled via quantum Monte Carlo, given that its values are the result of the fine-tuning procedure of the chemical potential required to achieve a desired average $N$. Figure 1 shows $\mu = \mu(V_t, N, \ldots)$ for different cases of the BH model without external potentials, $V_2 = 0$, and for an applied incommensurate superlattice potential with strength $V_2 = U$ and incommensurability parameter $\alpha = 0.7714 \ldots$ identical to that of the experiment of [12]. The behavior of $\mu$ for a commensurate superlattice with $\alpha = 3/4$ is found to be very close to that of the incommensurate case. In the case of weakly interacting bosons and taking the continuum limit of the lattice system, Thomas–Fermi (TF)

Figure 1. Scaling of the chemical potential $\mu$ for the 1d BH model in a parabolic trap (a), and in a trap plus an incommensurate superlattice potential with strength $V_2 = U$ (b). $\mu$, $V_t$, $V_2$ and $U$ are here reported in units of $J$. For all $N$ values, we have considered a broad range of trapping potentials $V_t/J$ from $4 \times 10^{-3}$ to 0.12. The dashed lines correspond to a linear fit to the high-$N$/high-$V_t$ data. The insets show that all curves exhibit a universal scaling of the slope.

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theory [23] would predict the following scaling for the chemical potential in \(d\)-dimensions:

\[
\mu \sim (NU)^{2/(2+d)} V_1^{d/(2+d)}
\]

which gives \(\mu \sim (NU)^{2/3} V_1^{1/3}\) for \(d = 1\). Figure 1 shows that, at fixed \(U\) and \(V_2\), and for all the cases considered, \(\mu\) is a homogeneous function of the combination \(x = N^{2/3} V_1^{1/3}\); in particular, even for large \(U/J\) ratios it surprisingly verifies the TF prediction of linear dependence on \(x\); significant deviations are observed only in the low-density and high-\((U/J)\) case, where lattice commensuration effects, not captured by the continuum TF approach, become significant, and where the hardcore boson regime sets in for density smaller than one\(^{1}\). Remarkably, for sufficiently high filling and/or trapping potential all the data for different \(U\)s and \(V_2\)s can be reproduced by a generalized TF scaling form

\[
\mu \approx (U/J)^{2/3} [C(U/J, V_2/J) + f_\mu(x)],
\]

where \(f_\mu\) is essentially a straight line, and \(C(U/J, V_2/J)\) is an offset term which depends weakly on the Hamiltonian parameters. Indeed, rescaling \(\mu\) by \((U/J)^{2/3}\) shows that all the \(\mu\) curves have essentially the same slope (insets of figure 1), and that the \(C\) offset leads to a slight deviation from the collapse onto a universal curve. A linear fit for the \(V_2 = 0\) data gives \(f_\mu(x) = 0.818(1)x, 0.818(2)x, 0.815(5)x\) and \(C = -1.234(6), -1.222(2), -1.32(4)\) for \(U/J = 5, 10\) and 20, respectively. We notice that the TF theory would predict \(f_\mu(x) = [3\Gamma(3/2)/(2\pi^{3/2})]^{2/3} = 0.825 48x\), which captures surprisingly well the \(x\)-dependent part of the numerical data.

Therefore, we obtain a universal prediction for the dependence of the effective chemical potential in the center of the trap on the experimentally controllable parameters \(J, U, V_1\) and \(N\) for a large range of their values, and for the extreme case of \(d = 1\) where the applicability of mean-field theory is in doubt. Similar results are obtained for the cases \(d = 2, 3\) and will be presented in a forthcoming publication. Hence we can firmly conclude that the chemical potential in the center of the trap represents a well-controlled experimental parameter.

 Armed with this prediction, we can then move on to simulate the outcome of a trap-squeezing experiment, where the central density \(n_C\) is monitored as a function of the trapping potential \(V_t\). We start from the case of the 1d BH model without any superlattice, for which we consider a boson number \(\langle N \rangle = 100\) in a variable-frequency trap and with fixed repulsion \(U/J = 20\). Figure 2 shows the evolution of the central density \(n_C\) averaged over a region \(C\) containing 10–20 sites as a function of the chemical potential \(\mu(V_t)\), and compared with the data for the bulk system. It is evident that, for a sufficiently low \(\mu\) (namely for sufficiently low \(V_t\)), the bulk density curve is very well reproduced (in this case for \(n_C \leq 2\)). The deviation of \(n_C\) from the bulk value reveals that the truly homogeneous region in the trap center has become smaller than the \(C\) region, a fact that can be simply cured by increasing the number of particles and decreasing the trapping potential so as to leave \(\mu \sim V_1^{1/3} N^{2/3}\) fixed. The succession of incompressible plateau regions at integer filling and compressible regions in the \(n_C(\mu)\) curve marks the alternation between incoherent MI and coherent superfluid (SF) behavior, as also revealed by the (global) coherent fraction \(n_{k=0} = (1/N) \sum_{ij} \langle b_i^\dagger b_j \rangle\). Remarkably, when the effective chemical potential in the trap center overcomes the Mott gap, a few particles can be transferred from the wings to the center into a locally SF state, and this gives rise to a violent increase in the coherent fraction with a very sharp kink. The width of the integer-filling plateaus

\(^{1}\) In this regime of low density and high \(U/J\) the behavior of the system becomes independent of \(U\) as observed in figure 1(a), given that multiple occupancy is essentially absent in the system. In the presence of a strong superlattice \(V_2 = U\), on the contrary, multiple occupancy persists at lower densities due to confinement of the particles in the superlattice minima. This explains the absence of the hardcore regime in the data of figure 1(b).
corresponds to that of the MI lobes in the phase diagram of the 1d BH model: hence this kind of measurement allows the phase diagram to be reconstructed with high accuracy, and the particle (hole) gap to be extracted at any point as the minimal chemical potential variation required to increase (decrease) the density. In particular, trap squeezing probes the density-driven transition from MI to SF, which is in a different universality class [1] with respect to the transition driven by the $J/U$ ratio and nominally probed so far in experiments [3, 15, 26]. Moreover, we emphasize the high tolerance of the method to the variation of the size of $C$, which corresponds to the size of the focus of the imaging laser.

Having shown that trap squeezing allows the phase diagram of the bulk BH model to be reconstructed, we generalize this approach to probe other phases of correlated bosons in an optical lattice. To this end, we consider $N = 100$ trapped bosons in an additional commensurate superlattice potential [24] with $\alpha = 3/4$, fixed phase $\phi = 0$ and strength $V_2 = U = 20J$, such that it overcomes the MI gap and hence removes the MI phase; the insulating phase that is left for large $U/J$ is a BI with fractional, commensurate fillings $(2n + 1)/4$ ($n = 0, 1, \ldots$). Figure 3 shows the alternation of phases in the center of the trap under trap squeezing as revealed by the central density, and compared to the bulk result; similarly to the MI–SF transition, the BI–SF alternation is clearly evidenced. The density plateaus correspond to the formation of incompressible BI region in the trap center, an event associated with a significant lowering of the global coherence in the system, as shown by the $n_{k=0}$ curve; the coherence is suddenly increased when the BI gap is overcome by the chemical potential and particles are transferred into a locally SF state in the center.

The situation changes drastically when tuning slightly the superlattice parameter from the commensurate value $\alpha = 3/4$ to the incommensurate value $\alpha = 0.7714\ldots$ realized in recent experiments [12]. In this case, for a strong superlattice $V_2 = U$ and for small $J/U$ the ground state of the system changes from SF to incompressible incommensurate band insulator (IBI) and
Figure 3. Central density and global coherent fraction for the 1d BH model in a trap and in a commensurate superlattice \((V_2 = U = 20J, \alpha = 3/4 \text{ and } \phi = 0)\). All symbols and notation as in figure 2. Notice that the deviation of the data for \(C = 10\) sites from the bulk ones is due to the fact that the \(C\) region does not contain an integer number of periods of the superlattice potential.

Figure 4. Central density and global coherent fraction for the 1d BH model in a trap and in an incommensurate superlattice \((V_2 = U = 20J\) and \(\alpha = 0.7714 \ldots)\); \(\langle \ldots \rangle_\phi\) denotes the average over fluctuations of the spatial phase \(\phi\). The boxes mark some relevant extended regions exhibiting BG behavior. All other symbols and notation as in figure 2.

to compressible BG upon changing the chemical potential \[19\]. Figure 4 shows the variation under trap squeezing for the central density averaged over random fluctuations of the spatial phase, \(\langle n_C \rangle_\phi\). This average is intrinsic in current experimental setups, where the phase \(\phi\) can change from shot to shot, and it is essential for the central region of the trap to sample the full statistics of the quasi-periodic potential and hence to mimic the bulk behavior of the system \[19\]. Indeed, we observe that \(\langle n_C \rangle_\phi\) reproduces very well the bulk behavior for low enough density. In
striking contrast to the previous two cases of no superlattice and of a commensurate superlattice, the \( \langle n_C \rangle \) curve exhibits extended compressible regions for which the coherent fraction does not vary upon changing the chemical potential. This corresponds to transfer of particles at no energy cost from the wings to the center of the trap into localized states which do not contribute to the coherent fraction of the system: this fact provides smoking-gun evidence for the appearance of a BG state in the center of the trap\(^2, 3\). Moreover, the joint information coming from the central density and the global coherent fraction enables experimental probing of the incompressible IBI behavior and the compressible SF behavior.

In summary, we have proposed an experimental method (trap squeezing spectroscopy) to directly extract bulk properties of strongly correlated bosons from measurements on a trapped system—a fundamental requirement in the future perspective of quantum simulations of complex quantum systems realized with cold atoms. The method relies on a simple, universal relationship between the trapping potential and the effective chemical potential for the particles in the trap center, which we numerically elucidate in the case of the BH model realized in optical lattices. Measuring the response of the central density in the trap to the variation of the trapping potential provides direct access to the compressibility of the infinite system, a piece of information which is not directly accessible to current experimental setups and which is crucial to extract the energy gap over the ground state of the Hamiltonian implemented in the system. The method offers the possibility to extract the phase diagram of the BH model with high resolution. Most remarkably, the joint measurement of the compressibility and of the coherent fraction (obtained via time-of-flight techniques [3]) provides clear evidence for the realization of a BG state in the center of the trap. We have demonstrated this property in the case of an incommensurate superlattice as recently realized in experiments [12], although the same technique can be applied to different realizations of random or pseudo-random potentials [8]–[11].

From the experimental point of view, this method requires the application of an extra dipolar trap whose strength can be controlled independently of that of the optical lattice, and the measurement of the optical depth of the cloud over a region of order \( \sim 10 \) wavelengths \( (\sim 10 \mu m) \) of the optical lattice in all three spatial directions. The measurements of the central density and of the coherent fraction cannot typically be performed in the same shot, so that special care is needed in maintaining the number of particles \( N \) fixed from shot to shot to achieve the same experimental conditions. This can be typically obtained by post-selecting only

\(^2\) An estimate of the experimental parameters [19] corresponding to the regions marked as BG in figure 4 at the lowest chemical potentials gives a trapping frequency \( \nu \approx 30–50 \) Hz for \(^{87}\)Rb in a one-dimensional optical superlattice: here we consider transverse standing waves of wavelength \( \lambda_1 = 830 \) nm and intensity \( V_\perp = 30E_r \), a longitudinal primary one (at \( \lambda_1 \)) of \( V_0 \approx 8.5E_r \) and a secondary one (at \( \lambda_2 = 1076 \) nm as in [12]) with \( V'_0 \approx 0.6E_r \) giving \( V_2 \approx U \approx 20J \) \( (E_r = h^2/2m \lambda_1^2 \) is the recoil energy). Hence, the observation of BG behavior is possible for a fully realistic set of parameters.

\(^3\) In figure 4 a sizable interval in chemical potentials is observed \( (1.9 \lesssim \mu \lesssim 2.25) \) in which the bulk system gives a tight alternation of IBI and BG phases, while the average central density in the trapped system is more smoothly varying, suggesting that a continuous BG phase is instead realized in the trap. One can regard this event from two viewpoints. On the one hand, the strong sensitivity of the bulk system to a slight change in the chemical potential in this region of the phase diagram is such that the central region of the trap is not in a unique local phase, and hence the system does not realize a bulk BG over a measurable spatial range. On the other hand, the incommensurate superlattice potential plus the parabolic trap realize locally a quasi-random potential with a richer spatial Fourier spectrum than that of the superlattice alone, so that a ‘trapped BG’ is indeed realized in this system [19].
those measurements with the same total $N$ in the trap. Finally, the stability of the central-density measurements should be ideally checked against progressive reduction of the measurement spot: if the measured average density becomes independent of the spot size (as appears to be the case for the low-density region of figures 2–4) the effect of the trap boundaries on the measurement is clearly irrelevant. In this case the measurement does not need any further validation coming from ab initio classical-simulation data, and a truly quantum simulation of a bulk system is realized.

After the completion and first posting of this paper, we became aware of an experiment on trapped fermions in optical lattices [27] probing the global compressibility of the atomic cloud via trap squeezing. A decrease in the global compressibility can reveal the formation of incompressible regions in the trap (such as MI regions [27]). Yet the global compressibility of an inhomogeneous system with finite intersite hopping is always finite due to the dilute tails of the cloud, and hence it cannot unambiguously tell apart, e.g., the occurrence of a BG phase from a Mott insulating one [28].

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