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# Coherence and spectral weight transfer in the dynamic structure factor of cold lattice bosons

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ABSTRACT

Ultracold atoms have been used to create novel correlated quantum phases allowing to address many solid-state physics problems using the quasi-particle concept, which is the foundation of our understanding of many-body quantum systems. For bosons, the simplest kinds of excited states involve two particles and they are connected to the dynamic structure factor $S(\mathbf{k}, \omega)$, measured using Bragg spectroscopy, similarly to the angle-resolved photoemission spectroscopy (ARPES) in solid state physics – a major tool in the study of high-$T_c$ cuprates. Calculation of $S(\mathbf{k}, \omega)$ requires a significant numerical effort to determine multidimensional convolutions of momentum and frequency dependent constituents functions, which we achieve using parallelized fast Fourier transform. As a result, we are able to show that spectral weight transfer between low and high energies is an intrinsic property of the strongly correlated Bose system in close analogy to the doped Mott-Hubbard electronic insulator. Furthermore, the appearance of sharp coherence peaks in the superfluid phase of the cold bosons closely resembles the formation of sharply defined quasiparticle excitations below $T_c$ in cuprates suggesting an intimate connection between the intrinsic nature of these seemingly different systems.

## 1. Introduction

Atomic gases trapped in optical lattice have become a powerful tool in the investigation of solid-state physics phenomena [1], behaving in many ways like strongly correlated electronic systems, e.g. superconductors. They allow accurate control over parameters of the system: tunnelling and interactions between atoms can be precisely tuned, while the geometry of the lattice can be modified in wide range. As a result, they constitute a clean environment for observation of many-body quantum effects not disturbed by lattice defects, or material imperfections: a key phenomenon in these systems being a quantum phase transition between phase coherent superfluid state and strongly localized Mott insulator, which is tuned by strength of interactions between atoms [2]. Similarly to their solid-state counterparts, ultracold gases require new experimental tools to characterize their quantum many-body states. Dynamics of atoms can be easily investigated using time-of-flight experiments, in which all trapping potentials are suddenly switched off allowing the atomic clouds to expand in gravitational field. Since it also turns off interactions between particles, the distribution of momenta becomes temporarily frozen and can be imaged by measuring spatial absorption of the expanded cloud. On the other hand, the excitation spectrum of the atomic gases confined to optical lattices can be measured using methods based on response to scattering of photons from the correlated atomic state, which have been implemented recently in the form of: radio-frequency spectroscopy [3,4], Raman spectroscopy [5] and Bragg spectroscopy [6–9]. They reveal the band structure of these systems, which can facilitate the comparison of quantum gas phases with their condensed-matter equivalents.

From the theoretical point of view, description of strongly interacting ultra-cold atoms in optical lattice is challenging. Lack of a dominant energy scale (both tunnelling and interaction energies are comparable) hampers perturbational approaches. As the central phenomenon is the quantum phase transition between phase-coherent and localized states, knowledge of the low-energy excited states of many-body systems is crucial. The simplest kinds of low-energy excited states for bosons involve two particles and are connected to the dynamical structure factor $S(\mathbf{k}, \omega)$. Since this quantity is both momentum and frequency dependent, it requires a theoretical description that properly includes spatial and thermal fluctuations. To this end, we use a combination of the quantum rotor approach and Bogoliubov theory to decouple problem of strongly correlated particles into formation of the superfluid amplitude and long-range phase coherence. The quantum rotor approach has been successfully applied for quantum phase transitions [10], phase transitions in spin glasses [11], superconducting and magnetic systems [12–14], and Josephson junction arrays

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[15]. It has been also used for systems of ultracold atoms in optical lattices and compared with quantum Monte Carlo calculations [16] or experimental results, e.g., on time-of-flight patterns [17,18] (quantum rotor approach supplemented by Bogoliubov theory). The key point of this approach is a representation of strongly interacting bosons as particles with attached “flux tubes” rendering boson a composite object. This introduces a conjugate U(1) phase variable which acquires dynamic significance from the boson-boson interaction. This phase variable is perfectly suited to the problem since it takes a definite value in ordered superfluid state. It is in contrast to the particle number representation, since the number of bosons in the superfluid phase is not a well-defined quantity. As a matter of fact, the phase and particle number variables are conjugates in quantum mechanics and in this context phase degrees of freedom represent good quantum number for the problem under study.

This allows us to determine the analytical expressions for the structure factor. Although they can be obtained in a closed form, their analysis requires a significant numerical effort due to convolved nature of the problem, which we solve using parallel fast Fourier transform. The remainder of the paper is as follows: in the following section we provide a theoretical background and brief presentation of the theoretical approach. In Section 3 we describe the numerical computations and present the results. Finally, we summarize in Section 4.

## 2. Theoretical background

Bosons in optical lattices usually display short-range interactions, and as a result they constitute a many-body system that is described by Bose-Hubbard model [19]. When the occupancy in higher bands can be neglected it is given by

$$\mathcal{H} = -t\sum_{\langle \mathbf{r}>\mathbf{r}'\rangle}(a_{\mathbf{r}}^{\dagger}a_{\prime\mathbf{r}} + h.\,c.) + \frac{U}{2}\sum_{\mathbf{r}} n_{\mathbf{r}}(n_{\mathbf{r}}-1) - \mu\sum_{\mathbf{r}} n_{\mathbf{r}}, \tag{1}$$

where $a_{\mathbf{r}}^{\dagger}$ is the boson creation ($a_{\mathbf{r}}$ - destruction) operator at a site $\mathbf{r} = 1,\ldots,N$ of a two-dimensional square lattice. The particle number operator is denoted by $n_{\mathbf{r}}$, while the chemical potential $\mu$ controls the total number of atoms in the lattice. Furthermore, $t$ is the hopping element and $U$ the on-site interaction. Both $t$ and $U$ are related to the optical lattice depth parameter, which can be tuned by the laser intensity. At zero temperature $T$ and for small $t/U$, the system remains in the Mott insulator incoherent phase, while as $t/U$ is raised phase transition to a superfluid state sets in with long range phase coherence [20].

As in solid state physics, one needs to characterize the quantum many-body states in ultracold gases. To identify these, we concentrate on the dynamic structure factor [21], which is defined as real-time boson density-density correlation function [22]:

$$S(\mathbf{k},\omega) = \sum_{\mathbf{r}} e^{i\mathbf{k}\mathbf{r}}\int dt e^{-i\omega t}\left\langle \tilde{n}_{\mathbf{r}}(t)\tilde{n}(0)\right\rangle, \tag{2}$$

where the angular brackets denote the ensemble average. For $k$=0, we have $n_{\mathbf{k}} = \sum_{\mathbf{r}} n_{\mathbf{r}}$ and $S(\mathbf{k}\omega)$ has a trivial contribution at $\omega$=0, which we dismiss by considering $\tilde{n}_{\mathbf{r}}(t) = n_{\mathbf{r}}(t) - \langle n_{\mathbf{r}}(t)\rangle$. In experiments it describes the response of the system to Bragg spectroscopy [6–9] in the linear regime whenever the energy $\omega$ of the Bragg perturbation matches the energy difference between two eigenstates of the Hamiltonian. The function $S(\mathbf{k},\omega)$ encapsulates relevant information about correlations and obeys particle conservation as well as sum rules. As we shall see, it plays an important role as it accounts for the spectral-weight transfer between low and high energies, which in solid state physics is an intrinsic property of a doped Mott-Hubbard insulator, when strong local correlations are considered [23]. In the context of bosons, it was analyzed mainly for low-dimensional systems, e.g. 1D [24–28]. In this work, we compute the dynamic structure factor of two-dimensional bosonic lattice systems in the regime of strong correlations. We implement the quantum rotor mapping of the Bose-Hubbard model [16] combined with the fast Fourier transform to track changes of $S(\mathbf{q},\omega)$ in the momentum-energy space and identify signatures of the different quantum phases. The structure factor can be conveniently obtained using Matsubara technique [29] from the “imaginary-time” $0<\tau<\beta$ ($\beta = 1/k_BT$) density-density correlation function

$$\chi(\mathbf{r},\tau) = -\langle \tilde{n}_{\mathbf{r}}(\tau)\tilde{n}(0)\rangle. \tag{3}$$

Employing the fluctuation-dissipation theorem one obtains continuation to real frequencies

$$S(\mathbf{k},\omega) = \left.\frac{2\,\mathrm{Im}\,\chi(\mathbf{k},\omega_m)}{1-e^{-\beta\omega}}\right|_{i\omega_m\to\omega+i0^+}. \tag{4}$$

Here, $\omega_m = 2\pi m/\beta$ is the Matsubara frequency ($m = 0, \pm 1, \pm 2, \ldots$). To proceed, we decompose the physical boson annihilation operator as

$$a_{\mathbf{r}}(\tau) = e^{i\phi_{\mathbf{r}}(\tau)}b_{\mathbf{r}}(\tau), \tag{5}$$

where $\phi_{\mathbf{r}}(\tau)$ is a fluctuating quantum rotor phase field, dual to the local bosonic density. By the above decoupling, the original Hubbard model (1) is mapped onto a free boson Hamiltonian self-consistently coupled to a unitary group U(1) quantum phase rotor model [30]. The key advantage of the quantum rotor representation is that the on-site interaction in the Hamiltonian (1) has been replaced in the Lagrangian of the model $L = \int_0^\beta d\tau(\mathcal{L}_0 + \mathcal{L}')$ by a simple kinetic term $\mathcal{L}_0$ for the phase field,

$$\mathcal{L}_0 = \sum_{\mathbf{r}}\left[\frac{\dot{\phi}_{\mathbf{r}}^2(\tau)}{2U} + i\frac{\overline{\mu}}{U}\dot{\phi}_{\mathbf{r}}(\tau)\right], \tag{6}$$

where $\dot{\phi} = \partial_\tau\phi$ and $\overline{\mu} = \mu + U/2$, while

$$\mathcal{L}' = -t\sum_{\langle\mathbf{r}>\mathbf{r}'\rangle}[e^{-i\phi_{\mathbf{r}}(\tau)+i\phi_{\mathbf{r}'}(\tau)}\overline{b}_{\mathbf{r}}(\tau)b_{\mathbf{r}'}(\tau) + h.\,c.] + \sum_{\mathbf{r}}[\overline{b}_{\mathbf{r}}(\tau)\partial_\tau b_{\mathbf{r}}(\tau) + (Un_b - \overline{\mu})n_{\mathbf{r}}(\tau)]. \tag{7}$$

Furthermore, we use the mean-field type decomposition of the hopping term, which couples the auxiliary complex bosons ($X\equiv b$) and rotor ($Y\equiv e^{i\phi}$) fields according to $XY \to \langle X\rangle Y + X\langle Y\rangle$. This reduces the Hamiltonian (1) to two uncoupled Hamiltonians for transformed bosons and U(1) rotors [31], while preserving spatial correlations in the Lagrangian (7).

The Lagrangian (6), (7) allows for two possible orderings: a disordered state without long-range phase coherence, and a long-range phase-coherent state given by the order parameter $\Psi \equiv \langle a_{\mathbf{r}}(\tau)\rangle = b_0\psi_0$, where

$$\psi_0 = \langle e^{i\phi_{\mathbf{r}}(\tau)}\rangle, \tag{8}$$

designates the phase coherence and $b_0 \equiv \langle b_{\mathbf{r}}(\tau)\rangle$ is the Bogoliubov amplitude, which is non-vanishing in the strong-coupling limit.

Within quantum rotor formulation, according to Eq. (5) we write the $a$-boson Green function as a product of $b$-auxiliary boson and phase Green functions [32], namely

$$G(\mathbf{r},\tau) \equiv -\langle a_{\mathbf{r}}(\tau)\overline{a}(0)\rangle = -G_b(\mathbf{r},\tau)G_\phi(\mathbf{r},\tau) \tag{9}$$

with

$$G_b(\mathbf{r},\tau) = -b_0^2 - \langle b'_{\mathbf{r}}(\tau)\overline{b}'(0)\rangle \tag{10}$$

and $b_{\prime\mathbf{r}}(\tau) = b_0 - b_{\mathbf{r}}(\tau)$. The Green function for the rotor field

$$G_\phi(\mathbf{r},\tau) = -\langle e^{i[\phi_{\mathbf{r}}(\tau)-\phi(0)]}\rangle, \tag{11}$$

defines the phase coherence order parameter (8) according to:

$$1-\psi_0^2 = \frac{1}{N\beta}\sum_{\mathbf{k},m\neq 0} G_\phi(\mathbf{k},\omega_m). \tag{12}$$

Given the auxiliary boson and phase correlation functions, we can