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David Clément, Nicole Fabbri, Leonardo Fallani, Chiara Fort, Massimo Inguscio. Bragg spectroscopy of strongly correlated bosons in optical lattices. *Journal of Low Temperature Physics*, 2010, 158 (1-2), <http://www.springerlink.com/content/uu8t6n256m206606/>. 10.1007/s10909-009-0040-7 . hal-00620050

HAL Id: hal-00620050

<https://hal.science/hal-00620050>

Submitted on 8 Sep 2011

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Bragg spectroscopy of strongly correlated bosons in optical lattices

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Using inelastic scattering of light (Bragg spectroscopy), we study the low-energy excitations of strongly correlated phases of ultracold bosons on the cross-over from correlated 1D superfluids to Mott insulators. As it is commonly performed in solid-state physics, the use of such a probe allows us to extract important information about the atomic many-body state. In particular we show that we can extract information about the dynamical structure factor $S(\mathbf{q}, \omega)$ and about the one-particle spectral function $A(\mathbf{q}, \omega)$ from the Bragg spectra. This technique could be extended to study more exotic correlated phases of ultracold atoms.

I. INTRODUCTION

Quantum many-body systems are physical systems in the degenerate quantum regime characterized by strong correlations between their components. The interactions between the large number of particles composing the system cannot be neglected *a priori*. In this context the knowledge of the low-energy excitations is crucial since they control the response to a weak perturbation and the thermodynamics at low temperatures. The description of the dynamics of strongly correlated systems in terms of low-energy excitations (*e.g.* using Green functions) is common in condensed matter physics [1].

From the experimental point of view, a crucial step consists in finding ways to measure the low-energy excitations of many-body systems. For instance the development of angle-resolved photoemission spectroscopy (ARPES) has played a major role in the study of high- T_c superconductors giving information about the one-particle spectral function [2]. More generally, scattering of light or particles has proved to be a useful tool to measure low-energy excitations and better characterize strongly correlated systems [3, 4].

For almost a decade now, ultracold atoms have been used to create correlated quantum phases from which solid-state physics problems can be addressed from a different perspective [5]. Apart from directly tuning the atom-atom interactions via Feshbach resonances, a common way to increase correlations between atoms consists in loading the gas in optical standing waves (optical lattices) [6]. Low-dimensional gases, Mott-insulating phases and disordered insulating states have been realized in experiments using optical lattices for bosonic or fermionic atoms [5]. As in solid-state physics, experimental tools are necessary to characterize these quantum many-body ultracold gases. The response to scattering processes in a similar manner to what is done in condensed matter physics is a natural candidate. Along those lines several techniques have been proposed consisting in scattering photons from the correlated atomic state and some of them have been implemented recently. They include radio-frequency spectroscopy [7, 8], Raman spectroscopy [9] and Bragg spectroscopy [10–13]

In this paper we present our recent experimental work

[12, 13] which consists in exploring correlated states of ultracold bosons by inelastic light scattering (Bragg spectroscopy). We measure the excitation spectra of 1D Bose gases in the correlated superfluid regime as well as in the Mott insulator regime, observing novel experimental signatures.

II. TWO-PHOTON BRAGG TRANSITION: A PROBE FOR LOW-ENERGY EXCITATIONS

As mentioned in introduction, the knowledge of the low-energy excited states of many-body systems is crucial. The simplest kinds of low-energy excited states involve either one or two particles of the many-body ground-state and they are respectively connected to the one-particle spectral function $A(\mathbf{q}, \omega)$ and the dynamical structure factor $S(\mathbf{q}, \omega)$. $A(\mathbf{q}, \omega)$ essentially describes the probability to remove a particle with momentum $\hbar\mathbf{q}$ and energy $\hbar\omega$ from the many-body ground-state and $S(\mathbf{q}, \omega)$ describes the probability of creating an excitation with momentum $\hbar\mathbf{q}$ and energy $\hbar\omega$ *within* the many-body system. As we will show later the inelastic scattering process we implement allows us to obtain information about these two quantities. Let us first recall their definition:

$$A(\mathbf{q}, \omega) = \frac{1}{\mathcal{Z}} \sum_{i,f} e^{-\beta E_i} |\langle \phi_f | \psi(\mathbf{q}) | \phi_i \rangle|^2 \delta(\hbar\omega + E_f + \epsilon(\mathbf{q}) - E_i)$$
$$S(\mathbf{q}, \omega) = \frac{1}{\mathcal{Z}} \sum_{i,f} e^{-\beta E_i} |\langle \phi_f | \psi^\dagger(\mathbf{q} - \mathbf{k}) \psi(\mathbf{k}) | \phi_i \rangle|^2 \delta(\hbar\omega + E_f - E_i)$$

where $|\phi_i\rangle$ (*resp.* $|\phi_f\rangle$) are initial (*resp.* final) many-body states of the system with corresponding energies E_i (*resp.* E_f), $\mathcal{Z} = \sum_i e^{-\beta E_i}$ being the partition function with $\beta = 1/k_B T$. The operator $\psi(\mathbf{q})$ creates a particle with momentum \mathbf{q} . The energy $\epsilon(\mathbf{q})$ is that of the final excited state out of the many-body wave-function.

Scattering of light by atoms in the Bragg regime refers to an inelastic scattering process of photons which couples two momentum states of the same internal atomic state. In the following we note $\hbar\omega$ the energy and $\hbar\mathbf{q}$ the momentum transferred to the gas by means of this two photon transition. In the regime of negligible spontaneous light scattering, the atom-light interaction is de-

scribed as a dipole potential $V = \hat{V}e^{i\omega t}$ that couples state α and state β of the single atom, with

$$\hat{V} \propto \int d\mathbf{r} \psi_{\beta}^{\dagger}(\mathbf{r})\psi_{\alpha}(\mathbf{r}) \Omega(\mathbf{r})e^{i\mathbf{q}\mathbf{r}} \quad (3)$$

where the operator ψ_{α} (*resp.* ψ_{β}^{\dagger}) annihilates a particle in state α (*resp.* creates a particle in state β) and Ω is the Rabi frequency of the atomic transition. The calculation of the scattering rate of photons requires considering all possible initial and final many-body states with momentum and energy conservation conditions[?]. In evaluating the response of the atomic system to scattering of light from Eq. 3, one can make use of the Fermi golden rule to write the scattering rate as

$$\frac{2\pi}{\hbar} \frac{1}{Z} \sum_{i,f} e^{-\beta E_i} |M_{i,f}|^2 \delta(\hbar\omega + E_f - E_i) \quad (4)$$

where the matrix element are calculated for the operator of equation Eq. 3

$$M_{i,f} \propto \int d\mathbf{r} \langle \phi_f | \psi_{\beta}^{\dagger}(\mathbf{r})\psi_{\alpha}(\mathbf{r}) | \phi_i \rangle \Omega(\mathbf{r})e^{i\mathbf{q}\mathbf{r}} \quad (5)$$

In the presence of an optical lattice, the two-photon Bragg transition can couple atomic states which belong to different energy bands of the optical lattice (see Fig. 1). We label the different bands by the integer $n = 1.. \infty$, $n = 1$ corresponding to the lowest-energy band.

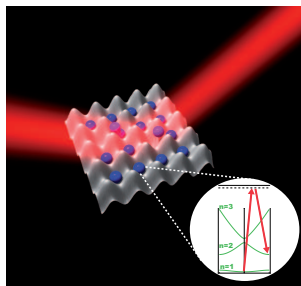


FIG. 1. (Color online) Artist's view of the experiment. A Mott insulating state of atoms (blue) loaded in optical lattices (grey) is shone with two laser beams (red) to excite the many-body system. Inset: Sketch of the two-photon Bragg transition in the optical lattice: atoms absorb from one Bragg beam and are stimulated to emit a photon in the second beam. The two-photon transition can excite the atom in any energy band, labelled n , of the optical lattice when the resonance condition on the energy and the momentum transferred is fulfilled.

We consider a two-photon transition from an atomic many-body state initially in the lowest-energy band ($n = 1$). We note the initial (*resp.* final) many-body wavefunction with N particles ϕ_i^N (*resp.* ϕ_f^N). We write $|\phi_i^N, N'_{n'}\rangle$ the state constituted of N atoms in the initial many-body wavefunction (*i.e.* in the lowest-energy band $n = 1$) and

N' atoms in a high-energy band $n' > 1$. With this notation a two-photon transition from the many-body ground state can take two forms:

- (i) it couples the state $|\phi_i^N, 0_{n'}\rangle$ to $|\phi_f^N, 0_{n'}\rangle$, *i.e.* the excited atom also belongs to the lowest-energy band $n = 1$;
- (ii) it couples the state $|\phi_i^N, 0_{n'}\rangle$ to $|\phi_f^{N-1}, 1_{n'}\rangle$, *i.e.* one atom is excited in the energy band n' .

We obtain two different types of contribution corresponding to the two elementary scattering processes (i) and (ii).

The matrix element for the first type of terms is:

$$|M_{i,f}|^2 \propto \left| \int d\mathbf{r} \Omega e^{i\mathbf{q}\mathbf{r}} \langle \phi_f^N, 0_{n'} | \psi_1^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}) | \phi_i^N, 0_{n'} \rangle \right|^2 \quad (6)$$

which can be rewritten as

$$|\langle \phi_f^N | \psi_1^{\dagger}(\mathbf{q} - \mathbf{k})\psi_1(\mathbf{k}) | \phi_i^N \rangle|^2. \quad (7)$$

By inserting it in the relation Eq. 4 one gets the relation defining the dynamical structure factor $S(\mathbf{q}, \omega)$ of the many-body state.

Terms of type (ii) correspond to the Bragg transition coupling a state in the lowest-energy band to a higher-energy band, $n' > 1$. Assuming that the *excited state is decoupled from the initial one*, one obtains

$$\begin{aligned} |M_{i,f}|^2 &\propto \left| \int d\mathbf{r} \Omega e^{i\mathbf{q}\mathbf{r}} \langle \phi_f^{N-1}, 1_{n'} | \psi_{n'}^{\dagger}(\mathbf{r})\psi_1(\mathbf{r}) | \phi_i^N, 0_{n'} \rangle \right|^2 \\ &\propto \left| \int d\mathbf{r} \Omega e^{i\mathbf{q}\mathbf{r}} \langle \phi_f^{N-1} | \psi_1(\mathbf{r}) | \phi_i^N \rangle \langle 1_{n'} | \psi_{n'}^{\dagger}(\mathbf{r}) | 0_{n'} \rangle \right|^2 \end{aligned} \quad (8)$$

which is proportional to

$$|\langle \phi_f^{N-1} | \psi_1(\mathbf{q}) | \phi_i^N \rangle|^2 \quad (10)$$

leading, after inserting into Eq. 4, to the one-particle spectral function $A(\mathbf{q}, \omega)$ of the many-body state[?]. When the Bragg process excites atoms from the Mott state to a high-energy band, assuming the initial and final states are independent is a good approximation. Indeed, being in the Mott regime implies that the amplitude of the periodic potential is large, *i.e.* that the different energy bands are separated by large energy gaps and that atoms in the many-body state are pinned at the lattice sites, resulting in a small overlap of the initial and final state wavefunctions. The same assumption would not hold in the superfluid regime for shallow lattice amplitudes where inter-band correlations might play a non-negligible role. In particular the result of Bragg scattering towards high-energy bands in the superfluid regime cannot be carried out in the simple way we use for the Mott state.

At last we note that the information about $S(\mathbf{q}, \omega)$ and $A(\mathbf{q}, \omega)$ related to the Mott state are distinguishable experimentally since they come from different energy scales in the excitation spectrum: while $S(\mathbf{q}, \omega)$ is

related to the response at low energies (typically $\omega/2\pi < 10$ kHz), $A(\mathbf{q}, \omega)$ is probed by measuring the excitation spectrum in higher-energy bands (corresponding to $\omega/2\pi > 30$ kHz).

III. EXPERIMENTAL PROCEDURE

The experiments are performed with ^{87}Rb atoms and the following time sequence [12, 13]. First, we load the ultracold atoms from a Bose-Einstein condensate (BEC) in three pairs of counter-propagating laser beams (optical lattices), the amplitudes of which determine the many-body state of the gas. Second, while the atoms are in this many-body state we shine them with two Bragg beams for a short duration (typically 3 to 6 ms) in order to create excitations in the system. Third, the amplitude of the optical lattices is ramped down to a small value ($5E_R$) where we wait for the excitations to thermalize. Finally, we switch both the 3D optical lattice and the magnetic trap, we let the atoms expand for a time-of-flight (typically 20 ms) and then we take an absorption picture of the atomic cloud. From the pictures we evaluate the energy absorbed by the atomic sample from the Bragg beams [12, 14]. Monitoring the energy absorbed as a function of the relative detuning ν between the Bragg beams, we obtain the excitation spectrum at a given momentum transfer $\hbar q_0$.

a. Creating correlated 1D Bose phases in optical lattices We create correlated atomic states using a 3D optical lattice ($\lambda_L = 830$ nm) with amplitudes along each axis scaled in recoil energy unit: $V_x = s_x E_R$, $V_y = s_y E_R$ and $V_z = s_z E_R$, where $E_R = \hbar^2/2m\lambda_L^2$ and m the atomic mass. All the experiments are performed with an array of 1D gases created by the lattices in the xOz plane, the amplitudes of which are fixed $s_x = s_z = s_\perp = 35$ and large enough to ensure the 1D character of the gases (the transverse trapping frequency is ~ 40 kHz much larger than the chemical potential $\mu_{1D} \sim 3$ kHz). Varying the amplitude s_y of the lattice along the axis of the 1D tubes, the gases are driven from a correlated superfluid state ($s_y = 0$) to a Mott insulating state ($s_y > 6$). Starting from a 3D Bose-Einstein condensate, the 3D optical lattice is adiabatically ramped up with a 140 ms-long exponential ramp with a time constant 30 ms. As already mentioned, after shining the Bragg beams, the 3D lattice is linearly ramped down to $s_\perp = s_y = 5$ where the system is left to thermalize for 5 ms. The expansion during a time-of-flight from the amplitude $5E_R$ leads to an interference pattern in the density distribution of atoms, the latter being the atomic equivalent of light diffraction on a grating [15].

b. Bragg beams setup The laser beams of the Bragg setup derive from a laser diode at $\lambda_B = 780$ nm and are typically detuned by 300 GHz from the atomic transition D_2 of ^{87}Rb . The resonant condition for the two-photon Bragg process depends on the energy and the momentum given by these two beams. The frequency difference

ν between the two beams (typically of the order of a few kHz) defines the energy transfer $\hbar\nu$ and it is controlled using two AOMs locked in phase. The momentum transfer $\hbar q_0$ is controlled by the angle θ between the beams, $q_0 = 4\pi/\lambda_B \sin(\theta/2)$. In the experimental setup, the two Bragg beams are controlled by independent mechanical supports which allows us to change θ . We align these mechanical setups in order to transfer the momentum $\hbar q_0$ along the axis of the 1D atom tubes. q_0 is calibrated using the well-known response of a 3D BEC in the absence of any optical lattice. The spectra presented in this paper have been measured at a fixed $q_0 = 0.96(3)k_L$ where $k_L = 2\pi/\lambda_L$.

c. Measuring the amount of excitations in the linear response regime The response of the gases to the Bragg excitation is monitored by measuring the energy absorbed by the atomic sample after thermalization of the excitations. In brief, we measure the width of the central peak in the interference pattern obtained in the atomic distribution after a time-of-flight, as discussed previously. We have checked that, when the two-photon Bragg process is resonant, the increase of this width is proportional to the energy absorbed by the atoms. In addition, this quantity increases linear with both the power and the duration of the Bragg pulse in the range of parameters we use (details can be found in [13]). Therefore the scattering of light at the finite momentum transfer q_0 we use allows exciting correlated atomic phases in a linear regime previously unaccessed by experiments.

IV. RESULTS

A. Dynamical structure factor $S(\mathbf{q}, \omega)$ of the many-body atomic state

As discussed in Sect. II, information about the dynamical structure factor $S(\mathbf{q}, \omega)$ of the many-body atomic state can be extracted from Bragg transitions within the lowest-energy band ($n = 1$) of the optical lattice V_y . When restricted to transitions within the lowest-energy band, the response of the 1D gases to the scattering of light is related to terms of the type $|\langle \psi_1^\dagger \psi_1 \rangle|^2$, *i.e.* to density-density correlation functions of the many-body state. In Fig. 2 we present low-energy Bragg spectra of the atomic gases across the superfluid to Mott insulator state. This cross-over is induced by increasing the amplitude s_y of the optical lattice along Oy , *i.e.* by changing the ratio $U/2J$ of the on-site interaction energy U over the next-neighbour hopping amplitude J [6].

d. Superfluid-Mott insulator cross-over The dynamical structure factor of a Mott insulating state is expected to be very different from that of a correlated superfluid [19]. This point is qualitatively enlightened by the spectra presented in Fig. 2. Indeed we observe that the Bragg spectrum of correlated 1D superfluids (Fig. 2a)), which exhibits a single broad resonance, is clearly distinguishable from the spectrum in the Mott

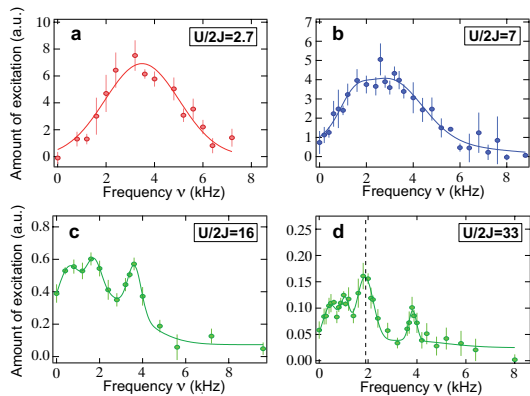


FIG. 2. Bragg spectra of the 1D gases across the superfluid to Mott insulator transition for four ratios $U/2J$ along the axis of the 1D atom tubes: 2.7 (corresponding to $s_y = 4$), 7 ($s_y = 7$), 16 ($s_y = 10$) and 33 ($s_y = 13$). The solid lines are guide to the eye. The vertical dashed line in d) marks the particle-hole excitation energy $\Delta_{p-h}(q_0)$. (Color online)

state (Fig. 2d)) where several narrow resonant peaks are observed. While the resonance of a 3D BEC is narrow [16], that of 1D superfluids is much larger due to the presence of stronger atom-atom correlations and temperature effects (thermal population of 1D phase fluctuations [17]). Concerning the Mott phase, we stress that the spectrum measured in the experiment is more complex than that of an homogeneous Mott insulator at zero temperature where a single resonance corresponding to a particle-hole excitation is expected. This complexity comes from: (i) the presence of a trapping potential which implies the existence of Mott regions with different fillings separated by superfluid domains (inhomogeneous Mott insulating state) [20]; (ii) the finite temperature of the system. We will discuss these points later in the paper.

More quantitatively, the appearance of the first Mott insulating region can be precisely located by monitoring the width of the broad resonance for low values of s_y (see Fig. 3a). The single resonance observed in the superfluid regime (Fig. 2a) presents a width which diminishes as s_y increases since the energy band flattens. When increasing s_y the 1D gases are driven into a state where a MI region appears with a resonant energy larger than that of the superfluid domain (the MI resonant energy lies above the lowest-energy band of the optical lattice $n = 1$). When the two peaks are not resolved, it implies that the width of the single resonance suddenly increases when a MI region appears. This analysis allows us to locate the appearance of the first MI region in the range $U/J = 8 - 10$ [12]. This estimate is in good agreement with the most recent Monte-Carlo calculations for trapped systems [18].

When the 1D gases are driven from a superfluid to an insulating state we expect the amplitude of the response to the light scattering to drop. The spectra in Fig. 2 clearly exhibit this behaviour. In addition, the amplitude is also expected to further drop in the MI state as the ratio U/J increases and atoms are more correlated. In

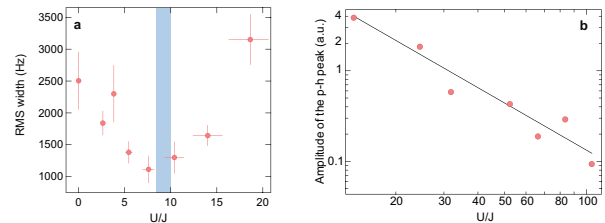


FIG. 3. **a** Evolution of the RMS width of the lowest-energy resonance across the superfluid to Mott transition. The shaded area corresponds to the theoretical prediction for the appearance of the first Mott region for our experimental parameters. **b** Amplitude of the response of a Mott state as a function of U/J at the frequency ν corresponding to the particle-hole excitation (see vertical dashed line on Fig. 2d). This amplitude scales as a power-law with the ratio J/U with an exponent 1.7(3). (Color online)

Fig. 3b we plot the amplitude of the peak located at the particle-hole excitation energy $\Delta_{p-h}(q_0)$ in the Mott state (see vertical dashed line on Fig. 2d). Fitting the experimental data with a power-law $(J/U)^p$ we find an exponent $p = 1.7(3)$ [21] in agreement with the expected value 2 [19].

e. Density-density correlations in the Mott state Elementary excitations in a homogeneous Mott-insulator state consist in particle-hole (p-h) excitations, *i.e.* moving a particle localized into a well of the periodic potential to a different site, already occupied. Therefore the typical energy needed for such a process is of the order of the on-site interaction energy U . The signature of the p-h excitations in the dynamical structure factor consists in a resonance located close to the energy U . As it appears on Fig. 2d) the largest resonant peak in the MI state (marked by a vertical dashed line) is observed at a frequency ~ 2 kHz which is close to the energy $U \simeq 2.2$ kHz. We have identified this resonant energy with the particle-hole excitation energy $\Delta_{p-h}(q_0)$ of the atomic Mott insulator for a momentum transfer $\hbar q_0$. In Fig. 4a) we plot $\Delta_{p-h}(q_0)$ as a function of U/J and we compare the measurement to the bare value U (solid line) calculated from the localized Wannier functions [5]. We observe a systematic downwards shift of $\Delta_{p-h}(q_0)$ compared to U . Δ_{p-h} is expected to converge towards U for $U/J \gg 1$ in the case of a homogeneous Mott insulator at zero temperature. In our experimental system, finite temperature effects and inhomogeneity might explain the observed discrepancy.

The presence of the trapping potential is responsible for the existence of several Mott and superfluid regions in the 1D gases [20]. In this inhomogeneous Mott-insulator state, a particle can hop to a site already doubly occupied. The resonant energy of this process is expected to be twice that of the homogeneous Mott resonant energy $\Delta_{p-h}(q_0)$. In Fig. 2d) a resonant peak is indeed present at a frequency ~ 4 kHz. We have plotted the ratio of this resonant energy (around 4 kHz) to the one identified as $\Delta_{p-h}(q_0)$ for different values of U/J in Fig. 4b): this

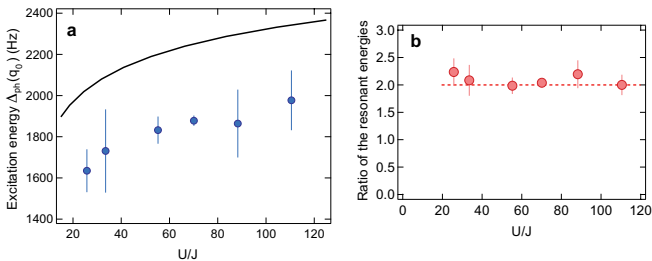


FIG. 4. **a)** Resonant energy of the particle-hole excitation $\Delta_{p-h}(q_0)$ as a function of the ratio U/J . The solid black line is the on-site interaction U . **b)** Ratio between $\Delta_{p-h}(q_0)$ and the next higher resonant energy. (Color online)

ratio is constant and equal to 2. We exclude non-linear processes since the response to the light scattering lies in the linear regime and we attribute the presence of the peak at $2\Delta_{p-h}(q_0)$ to the inhomogeneity of the experimental system (coming from the trapping potential and a loading in the optical lattice which might not be fully adiabatic).

Finally, we want to mention that we observed resonances in the energy range of 0.5-1.5 kHz in the Mott insulator regime (see Fig. 2d). These resonances can not be attributed to the superfluid domains since their energy is too high [12]. In an uniform Mott insulator, the energy difference between the ground-state and the p-h excitations is order of U while the energy splitting between the latter is of the order of J . The finite temperature of the system is expected to populate several p-h excitations on an energy scale of the order of the temperature, a property that can be probed using Bragg spectroscopy [19]. Further investigations have to be performed to compare the experimental signals around 1 kHz with this scenario.

B. One-particle spectral function in the Mott insulator

We now consider two-photon Bragg transitions towards high-energy bands ($n' > 1$) from an initial many-body state in the Mott insulator regime ($s_y > 6$). As mentioned in Sec. II, in this regime Bragg spectroscopy gives information about the one-particle spectral function of the many-body state since it involves terms like $|\langle\psi_1\rangle|^2$. This regime of coupling the many-body ground-state to high-energy single-particle states is analogous to techniques like ARPES in condensed-matter physics: the excited atoms in the high-energy bands are the equivalent to the removed electrons from the initial many-body state.

In Fig. 5 we present the measurement of a Bragg spectrum of an inhomogeneous MI state ($s_\perp = 35, s_y = 9$) in the energy range corresponding to excitations in the third band ($n' = 3$). A band-mapping technique has been used to measure the momentum of the excited atoms [15]. In this way we have demonstrated that the excitations pre-

sented in the energy scale of Fig. 5 indeed belong to the third energy band (see [13] for details).

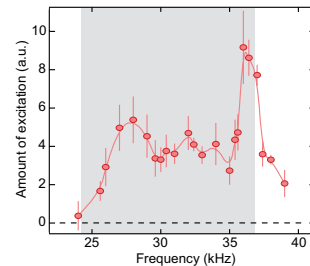


FIG. 5. Bragg spectrum of a Mott insulator ($s_\perp = 35, s_y = 9$) in the energy range corresponding to transitions towards the third energy band ($n' = 3$). The modulation of the observed amplitude on this energy scale might give information about the one-particle spectral function. The shaded area corresponds to the third energy band of single particles. (Color online)

The interesting feature in the spectrum depicted in Fig. 5 is the modulation of the amplitude in the response to the Bragg excitation. The interpretation of this point is currently under investigation and we expect it will give information on the one-particle spectral function of the Mott insulator as justified in Sec. II.

V. CONCLUSIONS

In this experimental work, we have implemented Bragg spectroscopy to probe the low-energy excitations in correlated quantum phases of ultracold bosons. We have shown how to measure the response of the atomic sample to the scattering of light in the linear regime. In such a regime the interpretation of the results are performed in close analogy with what is done in condensed matter physics. In particular, experimental observations can be thought in terms of the dynamical structure factor $S(\mathbf{k}, \omega)$ or the one-particle spectral function $A(\mathbf{k}, \omega)$. The experimental signatures of strong atomic correlations and their link to the dynamical properties of the many-body states of the gases have been enlightened. This point underlines the interest of using Bragg spectroscopy as a tool to probe low-energy excitations in correlated quantum atomic phases. This technique could easily be extended to more exotic experimental situations like correlated mixtures of different atoms where peculiar quantum phases are expected.

ACKNOWLEDGMENTS

We acknowledge E. Altman, S. Huber, M. Modugno and all the colleagues from LENS for stimulating discussions. This work has been supported by UE contract No. RII3-CT-2003-506350, MIUR PRIN 2007, Ente Cassa di

Risparmio di Firenze, DQS EuroQUAM Project, NAME-QUAM project and Integrated Project SCALA. This re-

search was supported by a Marie Curie Intra European Fellowship within the 7th European Community Framework Programme (D.C.).

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