Inelastic light scattering from a Mott insulator

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(Dated: March 22, 2022)

We propose to use Bragg spectroscopy to measure the excitation spectrum of the Mott insulator state of an atomic Bose gas in an optical lattice. We calculate the structure factor of the Mott insulator taking into account both the selfenergy corrections of the atoms and the corresponding dressing of the atom-photon interaction. We determine the scattering rate of photons in the stimulated Raman transition and show that by measuring this scattering rate in an experiment, in particular the excitation gap of the Mott insulator can be determined.

PACS numbers: 03.75.Hh, 67.40.-w, 32.80.Pj, 39.25+k

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Introduction. — A Bose-Einstein condensate in an optical lattice is a powerful new tool to investigate strongly correlated Bose gases [1]. In particular, the experiment by Greiner et al. [5] has shown that it is possible to achieve a quantum phase transition from a superfluid to a Mott-insulating phase by starting from an atomic Bose-Einstein condensate and loading this system into an optical lattice. This phase transition was predicted to occur in the Bose-Hubbard model by Fisher et al. [4], and Jaksch et al. [3] were the first to make the crucial observation that the Bose-Hubbard model can be applied to bosonic atoms in an optical lattice. A mean-field theory that describes the two phases of the Bose-Hubbard model was developed by van Oosten et al. [6].

An important advantage of using atoms in an optical lattice to study the Bose-Hubbard model, is that the system is free from disorder, which makes it possible to make very accurate predictions and measurements. A good example of such a high-precision measurement is Bragg spectroscopy. This technique has already been used to coherently split a Bose-Einstein condensate into two momentum components [7], to measure the excitation spectrum of a trapped Bose-Einstein condensate [8], and to measure the light-shifted energy levels of an atom in an optical lattice [9]. Here we propose to use Bragg spectroscopy to measure the excitation spectrum of the Mott-insulator state. In particular, one can in this way determine the value of the particle-hole gap in the excitation spectrum and study the behaviour of this gap as the system approaches the quantum critical point. Note that the excitation spectrum as obtained using Bragg spectroscopy will not yield what is generally referred to as the Mott gap, because this gap is associated with single-particle excitations. The value of the particle-hole gap is an interesting quantity in the study of quantum critical phenomena, but it is also very important for the practical application of these systems in quantum information processing, since the gap determines the fidelity of the Mott state. It is important to realize that the system of a Bose-Einstein condensate in an optical lattice is more complicated than the above mentioned systems, because in this case many-body effects and strong correlations have to be taken into account. In a Bragg spectroscopy experiment, two laser beams are used to make excitations in the system, as shown in Fig. 1(a). The two lasers both have a large detuning with respect to an optical transition in the atoms so that spontaneous emission is suppressed. However, the relative detuning can be very small. When an atom absorbs a photon from beam two and is stimulated to emit a photon into beam one, the atom undergoes a change of momentum $\hbar q = \hbar k_2 - \hbar k_1$ and a change of energy $\hbar \omega = \hbar \omega_2 - \hbar \omega_1$. In principle any optical transition could be used, but here we use the same transition that is employed to create the lattice potential. This means that the magnitude of the momentum is given by $\hbar q = 2\hbar k_{\text{ph}} \sin(\theta/2)$, where to a good approximation $\hbar k_{\text{ph}} = 2\pi \hbar / \lambda$ is the photon momentum of both the lasers, $\lambda$ is equal to the wavelength of the lattice laser light and $\theta$ is the angle between the two laser beams. By varying the angle between the two laser beams, any momentum between zero and $2\hbar k_{\text{ph}}$ can be transferred and by varying the relative detuning between the beams, the amount of energy that is transferred to the system can
be controlled. Calculating the scattering rate for a given momentum \( hq \) and energy \( \hbar \omega \) roughly speaking involves counting the number of ways in which the requirements of momentum and energy conservation can be met. To illustrate this process, we draw in Fig. 1(b) the quasiparticle and quasihole dispersions in the Mott insulator \( \mathcal{D} \), as is common in solid-state physics. The horizontal and vertical arrows in the figure indicate the transfer of momentum and energy respectively. Since energy is deposited in the system, this scattering rate can be measured in a trapless experiment, or by determining the increase in temperature of the medium. The polarizibility can be written as 
\[
\chi(q, \omega) = \frac{1}{2} \int_{1BZ} dq \frac{P(k, k + q, \omega)}{-h \omega^+ + \epsilon^\text{qp}(k + q) - \epsilon^b(k)},
\]
and the time-reverse process can be written as 
\[
\chi_\omega^0(q, \omega) = \chi_\omega^0(-q, -\omega).
\]
This equation contains the probability \( P(k, k + q, \omega) = (1 - Z(k)) Z(k + q) \) for the creation of a hole with momentum \( k \) and a particle with momentum \( k + q \), and an energy denominator that is associated with the energy cost \( \epsilon^\text{qp}(k + q) - \epsilon^b(k) \) of that process. This can readily be verified by taking the imaginary part of the susceptibility, which is proportional to 
\[
\int_{1BZ} dq \frac{P(k, k + q, \omega) \delta(h \omega - \epsilon^\text{qp}(k + q) + \epsilon^b(k))}{-h \omega^+ + \epsilon^\text{qp}(k + q) - \epsilon^b(k)}
\]
and can be understood as Fermi's Golden Rule. The actual computation of the above integral is too complicated to do analytically, so that we have to resort to numerical methods. We achieve this by calculating the imaginary part of the susceptibility using the Greens function in Eq. (2), which roughly corresponds to integrating over the surface in the Brillouin zone where the energy denominator vanishes. In practice, this amounts to numerically finding the poles of the expression and determining their residue. The real part is calculated from the imaginary part using a Kramers-Kronig relation.

However, the results that one would obtain in this manner do not obey particle conservation. Physically, a Raman process with momentum \( q \) couples to a density fluctuation \( \rho(q) \). For zero-momentum transfer, \( \rho(0) \) corresponds to the total number of particles and fluctuations are impossible due to particle-number conservation. If we compute the imaginary part of Eq. (4) for \( q = 0 \) we find a spectrum which is nonzero, which means that this approach is not sufficiently accurate. The problem is due to the fact that in Eq. (2) not the bare atomic propagator is used, but a dressed propagator which contains a large self-energy correction given by
\[
\hbar \Sigma(k, \omega) = 2N_0U + \frac{N_0(N_0 + 1)t^2}{\hbar \omega + U + \mu}.
\]
an atom moving through the Mott insulating background is dressed by all the other atoms. As is known from quantum field theory [11], one has to be careful when applying self-energy corrections to the calculation of the susceptibility, because in general these corrections do not obey the required conservation laws (in this case particle-number conservation). Using field-theoretical methods, we can derive so-called Ward identities, that show that every self-energy correction requires a corresponding vertex correction in order to restore the conservation laws. Physically this means, that if the atom is dressed, we also have to dress the atom-photon correction in order to restore the conservation laws. Diagrammatically this is illustrated in Fig. 2. This situation is very analogous to the situation in a superconductor, where the naive BCS calculation of the electro-magnetic response is not gauge invariant and a more involved approach is needed [12]. Using the relevant Ward identity [10] we can derive that the intuitive probability function given above, has to be replaced by

$$P(k; k + q, \omega) = \frac{2\hbar\omega - \epsilon_{mp}(k + q) + \epsilon_{nb}(k)}{\hbar\omega(k + q) + \hbar\omega(k)} \times (Z(k + q) - Z(k)). \quad (6)$$

Note that the probability now vanishes when $q \to 0$, so that particle conservation is indeed no longer violated. In fact, we can show that for small $q$ and $\hbar\omega$ just above threshold $P \propto q^2/\Delta_0^2$, where $\Delta_0$ is the gap for particle-hole excitations.

The imaginary part of Fig. 3 clearly shows singularities around $\hbar\omega = U$. These singularities are due to the fact that there are saddle points in the dispersion and that a saddle point in the dispersion causes an integrable singularity in the density of states. These are so-called van Hove singularities [13]. It is interesting to see, that the van Hove singularities split up as the momentum is increased, which is caused by the fact that the saddle-point energy in the direction of $q$ and the saddle-point energy in the orthogonal direction(s) are shifted by different amounts. This is also visible in Fig. 4. However, it is less clear in this case, because the van Hove singularities are more smeared out in three dimensions. Also, the opening of the threshold for the two-photon absorption in the three dimensional case is far less steep than in the two-dimensional case. To investigate possible collective modes in this system, we determined higher-order corrections in the random-phase approximation (RPA). It can be shown that in RPA the susceptibility is given by

$$\chi(q; \omega) = \chi^0(q; \omega)/(1 - U\chi^0(q; \omega))).$$

This means that there is a resonance in the scattering rate when the real part of $\chi^0(q; \omega)$ is equal to $1/U$. However, as can be seen from Figs. 3 and 4 the real parts in both cases are rather small compared to $1/U$ and in practice, including the RPA denominator does not qualitatively change our previous results.

In Fig. 5 we plot the imaginary part of $\chi_0$, for a range of values for the coupling constant $U/zt$, and for a fixed momentum $q = 0.10$. We see, that the threshold behaviour becomes steeper as we approach the critical value of $U_c/zt \approx 5.83$. We also see that there remains a nonzero gap when $U = U_c$. This is due to the fact that we are not considering a zero momentum excitation, due to the reasons given above. In the inset of Fig. 5 we plot this gap $\Delta_q$ as a function of $U/zt$. For large $U$ the gap grows

**Results. —** In Figs. 3 and 4 the result of a numerical integration is shown in two and three dimensions, respectively. Both calculations have been carried out for a regular square lattice and the momentum $q$ is chosen a principal lattice direction. All energies in the following figures are given in units $zt$, where $z$ is the coordination number of the lattice.
linearly with $U$ and for $U$ close to $U_c$, the gap closes more rapidly. In the case of $q = 0$ the gap would in our mean-field approximation close as $\sqrt{U - U_c}$ when $U \downarrow U_c$, but for small nonzero $q$ it closes as $\sqrt{U - U_c} + \eta q^2$, where the factor $\eta$ is a positive function of $U_c$ and $t$.

**FIG. 5:** Imaginary part of the susceptibility in a three-dimensional lattice for $q = 0.10$ along a lattice direction and $U/zt = 5.83, 7.8, 9, 10$

**Discussion.** — In summary, we have proposed a means of studying Mott insulators in optical lattices, using the relatively well-known technique of Bragg spectroscopy. We have presented spectra that can be measured directly by trap loss or heating measurements. In a recent experiment by Stöferle et al. [14] the authors use a setup where the laser beams are perfectly counterpropagating, which corresponds to a quasi-momentum transfer of zero. As we have argued above, there should be no scattering in that case and the signal can only be due to nonlinear response or to the fact that the system is inhomogeneous and of finite size. We have found that by measuring the threshold behaviour of the two-photon scattering rate at various quasi-momenta, it is possible to determine the gap by extrapolation. We have shown that for a theoretical description of Bragg spectroscopy on the Mott insulator it is absolutely essential to dress the photon-atom coupling, which is in a way unexpected, as the corrections are zero in the case of a harmonically trapped gas. As a result it turns out that although it is common to use the language of solid-state physics to describe these systems, the physics is qualitatively very different due to the many-body effects.

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