Bragg spectroscopy of ultracold atoms loaded in an optical lattice

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(Received 17 December 2004; published 12 August 2005)

We study Bragg spectroscopy of ultracold atoms in one-dimensional optical lattices as a method for probing the excitation spectrum in the Mott-insulator phase, in particular the one-particle-hole excitation band. Within the framework of perturbation theory we obtain an analytical expression for the dynamic structure factor $S(q,\omega)$ and use it to calculate the imparted energy which was shown to be a relevant observable in recent experiments. We test the accuracy of our approximations by comparing them with numerically exact solutions of the Bose-Hubbard model in restricted cases and establish the limits of validity of our linear-response analysis. Finally we show that when the system is deep in the Mott-insulator regime, its response to the Bragg perturbation is temperature dependent. We suggest that this dependence might be used as a tool to probe temperatures of order of the Mott gap.

DOI: 10.1103/PhysRevA.72.023407 PACS number(s): 32.80.Pj, 03.75.Hh, 03.75.Lm

I. INTRODUCTION

Recently, there has been a lot of experimental progress studying cold atoms confined in optical lattices. The defect-free nature of the lattice potential, the long coherence times of the constituent atoms, and the high experimental control of the lattice parameters [1,2] make this a unique system for precisely studying many-body physics. In particular, the experimental observation of the superfluid to Mott insulator quantum phase transition [3] has stimulated much interest in this area of research.

Perhaps one of the most important potential applications of the Mott-insulator transition is to use it as a means to initialize a quantum computer register [4–7]. Particularly in this case, it is important to have tools for thoroughly characterizing the experimentally obtained Mott-insulator states. The usual procedure for entering the Mott-insulator regime is to begin with a magnetically trapped Bose-Einstein condensate (BEC) (with almost all the atoms in the condensate), and slowly load it into an optical lattice by increasing the lattice depth. One key piece of evidence for the quantum phase transition is the loss of global phase coherence of the matter wave function when the lattice depth increases beyond a critical value [3]. However, the loss of coherence could arise from many sources, such as the decoherence induced by quantum or thermal depletion of the condensate during the loading process [8] and therefore it is not a sufficient signature that the system is in the Mott-insulator state. For this reason, in the experiments by Greiner *et al.* [3], complementary evidence for the Mott-insulator transition was provided by applying a potential gradient to the lattice to show the presence of a gap in the excitation spectrum. In this paper we show that Bragg spectroscopy, done by applying additional laser beams independent from the lattice beams, is an experimental technique with the potential to thoroughly characterize the Mott phase. In addition to determining the energy gap, we show that it provides detailed information about the excitation spectrum, information unavailable using other techniques. Moreover, in contrast to applying a potential across the lattice Bragg spectroscopy is not susceptible to effects like Bloch oscillations and Zener tunneling. Furthermore, we show that unlike in the superfluid regime, the system's response to Bragg perturbation in the Mott regime is sensitive to finite temperature. This property might be used as a tool to probe temperatures of order of the Mott gap.

Our analysis is based on a perturbative treatment, which we show to be applicable in the strong Mott regime that has been reached in current experiments [9]. Although our approach is applicable only in the range of validity of first-order perturbation theory, it has the advantage of properly including one-particle-hole correlations. Such correlations have a dominant influence on the spectrum of the system and are not accounted for in mean-field treatments [10].

The organization of this paper is the following. In Sec. II we introduce the basic formalism that describes Bragg spectroscopy in an optical lattice and use a linear-response approach to calculate the imparted energy to the system. In Sec. III we derive the zero-temperature response to Bragg spectroscopy of a translationally invariant lattice deep in the Mott regime and in Sec. IV we discuss the conditions required for our linear-response analysis to be valid. In Sec. V we extend the zero-temperature analysis to finite temperature and finally in Sec. VI we conclude.

II. FORMALISM

The typical Bragg spectroscopic procedure is to gently scatter atoms in an ultracold gas system with a moving potential of the form $V_0\cos(qx-\omega t)$. This type of experiment was first demonstrated by Stenger *et al.* [11] and Stamper-Kurn *et al.* [12]. In contrast to earlier experiments that used momentum as the response observable, here we choose to examine the imparted energy. In trapped systems this allows long excitation duration which facilitates more precise spectral resolution. Energy spectroscopy is not as well developed as momentum spectroscopy but recent experiments have demonstrated the use of this technique [13]. The Bragg

potential is formed by the ac Stark shift arising from a pair of interfering light fields (e.g., see [14]). In this paper we will always assume that the Bragg potential is *generated independently* of and is much weaker than the lattice potential. We therefore treat the scattering process with linear-response theory. Using an independent set of beams to generate the Bragg potential also provides considerable flexibility in the range of q and ω values that can be obtained.

In this work we consider one-dimensional (1D) bosons loaded in an optical lattice. Effective 1D systems have been realized in recent experiments (for example Refs. [9,13]) by loading a Bose-Einstein condensate into a three-dimensional optical lattice, which is very deep in two directions. The dynamics is then restricted to the third, or axial, direction only. In this work we study the response of the system to Bragg perturbation in the axial direction, assuming that the dynamics in the transverse directions is frozen. We consider a one-dimensional optical lattice which is sufficiently deep that the tight-binding approximation is valid and assume that we can restrict the dynamics of the atoms to the lowest vibrational band. This applies when changing the lattice potential does not induce band excitations. This condition is satisfied when the frequency ω of the Bragg perturbation is less than the gap between the first and second bands, and when the momentum transfer q is contained within the first Brillioun zone. A detailed analysis of the validity of this first-band approximation to study Bragg scattering of a dilute weakly interacting gas in an optical lattice is found in [15] where the authors used a mean-field approach combined with Bogoliubov analysis. In the single-band approximation and in absence of external potentials, the system is described by the Bose-Hubbard Hamiltonian (BHH) [16]

$$\hat{H} = -J\sum_{\langle n,l\rangle} \hat{a}_n^\dagger \hat{a}_l + \frac{U}{2}\sum_n \hat{a}_n^\dagger \hat{a}_n^\dagger \hat{a}_n \hat{a}_n. \tag{1}$$

Here $\hat{a}_n$ is the annihilation operator at site n which obeys the canonical commutation relations for bosons, J is the hopping matrix element between nearest neighbors, and U is the on-site repulsion energy. The sum $\langle n,l\rangle$ is taken over nearest neighbors. We use N for the total number of atoms and M for the total number of wells. In the tight-binding approximation the Hamiltonian describing the Bragg perturbation reads

$$\hat{H}_B = \frac{1}{2}V_0(\hat{\rho}_q^\dagger e^{-i\omega t} + \hat{\rho}_q e^{i\omega t}), \tag{2}$$

where the density fluctuation operator $\hat{\rho}_{q_*}^\dagger$ is defined as $\hat{\rho}_{q_*}^\dagger = \Sigma_{n,m=0}^{M-1} I_q^{n-m}\hat{a}_m^\dagger \hat{a}_n e^{iqmd}$, where $I_q^n = \int dx\, e^{iqx}\phi_0^*(x)\phi_0(x-dn)$ is a geometrical factor that involves integration over Wannier functions $\phi_0(x)$, and d is the lattice constant. For deep lattices $I_q^n \propto \delta_{n,0}$ [15].

To analyze the Bragg spectrum of the system we study the energy transfer, which can be measured by time-of-flight techniques [13]. Under linear-response theory, the energy transfer is related to the so-called *dynamic structure factor* $S(q,\omega)$, which is given by

$$S(q,\omega) = \frac{1}{\mathcal{Z}}\sum_{ij} e^{-\beta E_i} f_q(\omega_{ij}), \tag{3}$$

where $f_q(\omega_{ij}) \equiv |\langle i|\hat{\rho}_q|j\rangle|^2 \delta(\omega-\omega_{ij})$, $|i\rangle$ and E_i are eigenstates and eigenenergies of the unperturbed Hamiltonian (1), $e^{-\beta E_i}$ is the usual Boltzmann factor with $\beta = 1/k_B T$ where k_B is Boltzmann's constant and T the temperature, $\mathcal{Z}$ is the canonical partition function, and $\hbar\omega_{ij} = E_j - E_i$. Because of the factor $f_q(\omega_{ij})$, the system's response shows peaks whenever the frequency of the Bragg perturbation matches the energy difference between two eigenstates of the BHH. The peak height is proportional to the the transition probability between the two eigenstates, $|\langle i|\hat{\rho}_q|j\rangle|^2$.

The total energy transfer after applying the Bragg perturbation can be shown to be given by [17]

$$\delta E = \frac{V_0^2}{2\hbar}\int_0^{T_p} dt \int_{-\infty}^{\infty} d\omega'\,\omega'\chi(q,\omega')\frac{\sin[(\omega-\omega')t]}{(\omega-\omega')}, \tag{4}$$

where T_p is the duration of the perturbation and $\chi(q,\omega) = S(q,\omega) - S(-q,-\omega)$. Here we derive analytic expressions for the dynamic structure factor assuming we are deep in the Mott-insulator regime, where treating the hopping term in the Hamiltonian as a perturbation is justified.

III. ZERO-TEMPERATURE RESPONSE

In this work we assume a commensurately filled lattice with no external confinement, filling factor $N/M = g$, and periodic boundary conditions. The unperturbed Hamiltonian includes only the on-site interaction term, which is diagonal in a number Fock-state basis. To zeroth order the ground state $|\Phi_0^{(0)}\rangle$ is the Fock state with g atoms in every lattice site. The lowest-lying excitations correspond to the one-particle-hole (1ph) states $|\Psi_{mn}\rangle$ with $g+1$ particles at site m, $g-1$ particles at site n, and exactly g particles in every other site. There are $M(M-1)$ 1ph excitations and, because of the translational symmetry, they are degenerate at zeroth order with excitation energy U. To zeroth order the dynamic structure factor vanishes. At first order the ground-state wave function is $|\Phi_0^{(1)}\rangle = |\Phi_0^{(0)}\rangle + J/U\sqrt{2Mg(g+1)}|S\rangle$, where $|S\rangle \equiv \Sigma_{n=1}^{M}(|\Psi_{nn+1}\rangle + |\Psi_{nn-1}\rangle)/\sqrt{2M}$ is the normalized translationally invariant state of adjacent particle-hole excitations. In order for perturbation theory to be valid, the parameter $Jg\sqrt{M}/U$ has to be small [7]. This could be a significant restriction for systems with a large number of filled sites but can be perfectly realized in experiments such as Ref. [9] where the system has only 20 occupied sites in the central tube. To find first-order corrections to the $M(M-1)$ low-lying excited states we must diagonalize the kinetic energy Hamiltonian within the 1ph subspace. If we expand the eigenstates as a linear combinations of 1ph excitations $|\Phi_i^{(1)}\rangle = \Sigma_{n,m\neq n} c_{nm}^i |\Psi_{nm}\rangle$ the necessary and sufficient conditions that the coefficients c_{nm}^i have to satisfy are

$$(g+1)(c_{n+1m}^i + c_{n-1m}^i) + g(c_{nm+1}^i + c_{nm-1}^i) = \tilde{E}_i c_{nm}^i, \tag{5}$$

with $E_i^{(1)} = U - J\tilde{E}_i$. In addition to Eq. (5), the amplitudes c_{nm}^i have to satisfy periodic boundary conditions $c_{n+Mm}^i = c_{nm+M}^i$

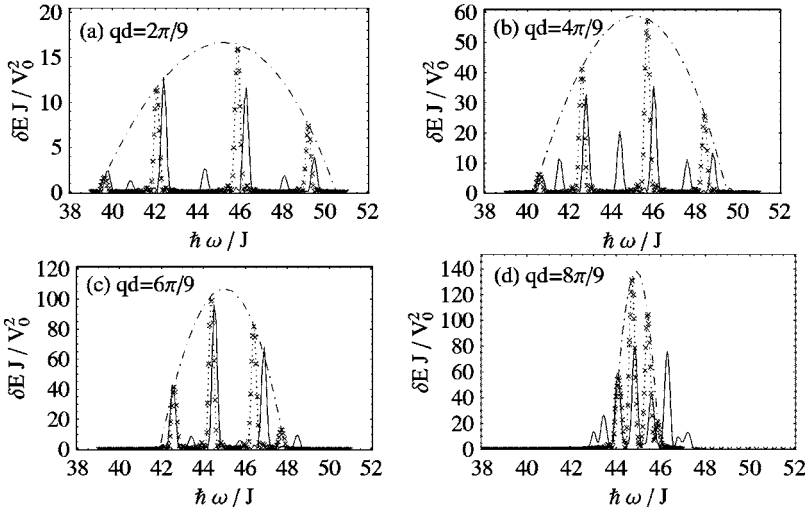

FIG. 1. Energy transfer for a homogeneous system at zero temperature. Solid line, exact solution; crosses, perturbative solution (envelope, dashed line). Other parameters: $M=N=9$, $J\tau/\hbar=20$, $U/J=45$.

$=c^i_{nm}$ and the constraint $c^i_{nn}=0$ (which prevents particle and hole excitations occurring at the same site). Equation (5) is analogous to the tight-binding Schrödinger equation of a two-dimensional square lattice in the xy plane. The x direction is associated with the position of the extra particle and the y direction with the position of the hole. The different weights $g+1$ and g can be understood in the 2D lattice model as different effective masses in the two directions and the constraint $c^i_{nn}=0$ as a hard wall along the $x=y$ line. The solutions are not straightforward due to the fact that the effective-mass difference breaks the lattice symmetry around the $x=y$ axis and makes the hard-wall constraint hard to satisfy. However, in the limiting case of high filling factor $g \gg 1$, the solutions of Eq. (5) (including the constraints) are

$$E^{(1)}_{rR} = U - 2J(2g+1)\cos\left(\frac{\pi r}{M}\right)\cos\left(\frac{\pi R}{M}\right), \tag{6}$$

$$c^{r,R\neq 0}_{nm} = \begin{cases} \dfrac{2}{M}\sin\left(\dfrac{\pi r}{M}|n-m|\right)\sin\left(\dfrac{\pi R'}{M}(n+m)+\alpha_{rR}\right), \\ \dfrac{2}{M}\sin\left(\dfrac{\pi r}{M}(n-m)\right)\sin\left(\dfrac{\pi R''}{M}(n+m)+\beta_{rR}\right), \end{cases} \tag{7}$$

$$c^{r,0}_{nm} = \begin{cases} \dfrac{\sqrt{2}}{M}\sin\left(\dfrac{\pi r}{M}|n-m|\right), & r \text{ odd}, \\ \dfrac{\sqrt{2}}{M}\sin\left(\dfrac{\pi r}{M}(n-m)\right), & r \text{ even}, \end{cases} \tag{8}$$

where we used $i=(r,R)$, with $r=1,\ldots,M-1$ and $R=0,\ldots,M-1$. The notation R' restricts the values of R to the ones where $R+r$ is an odd number and R'' to the values where $R+r$ is even. The constants $\alpha_{rR}=\pi(r-R+1)/4$ and $\beta_{rR}=\pi(r+R-1+M)/4$ guarantee the orthogonality of the eigenmodes.

Using Eqs. (6) and (8) we get an expression for the zero-temperature dynamic structure factor given by

$$S_0(q,\omega) = \frac{J^2}{U^2}g(g+1)\sum_{r,R}\delta(\omega - E^{(1)}_{rR}/\hbar)\left|\sum_{m=1}^{M} e^{iqdm}H^{rR}_m\right|^2$$
$$= 32\frac{J^2}{U^2}g(g+1)\sin^2\left(\frac{qd}{2}\right)\sum_r{}'\sin^2\left(\frac{\pi r}{M}\right)\delta\left(\omega - \frac{E^{(1)}_{r\tilde{q}}}{\hbar}\right), \tag{9}$$

where $H^{rR}_m = c^{rR}_{mm+1} + c^{rR}_{mm-1} - c^{rR}_{m+1m} - c^{rR}_{m-1m}$, $qd = 2\pi\tilde{q}/M$, and $\tilde{q}$ an integer between 0 and $M-1$. The prime in the sum imposes the constraint that $\tilde{q}+r$ is even. It is important to emphasize that only the states with $R=0$ have a dispersion relation which agrees to first order in J with the mean-field solution found in Ref. [10]. However, for these states $H^{r0}_m = 0$.

In Fig. 1 we compare the energy transfer as a function of the Bragg frequency calculated from Eq. (9) to results obtained by the exact diagonalization of the BHH for two values of Bragg momenta q. In contrast to the superfluid regime [15], where Bragg spectroscopy excites only the quasiparticle state with quasimomentum q, in the Mott regime we observe $M-1$ peaks pertaining to the two-dimensional character of the 1ph dispersion relation. The Bragg momentum q fixes one quantum number R but the other can take $M-1$ different values. In the analytic solution due to the constraint in Eq. (9), $\tilde{q}+r$ even, only $(M-1)/2$ of the possible $M-1$ peaks are present. The constraint is a consequence of the extra symmetry introduced in the high-filling-factor approximation where similar "effective masses" are assumed.

In the analytic solution, Bragg peaks have an overall envelope of the form of an inverted parabola centered at the gap energy U, with a maximum height proportional to $\sin^2(qd/2)$ and extended over an interval with an approximated width of $4J(2g+1)\cos(qd/2)$. The $\cos(qd/2)$ dependence of the width and $\sin^2(qd/2)$ dependence of the height indicate that as q approaches π/d the energy transfer is highly peaked around U. This behavior is observed in Fig. 1, where the overall width decreases as q approaches π/d, while the peak height increases. In spite of the fact that the analytic solution uses the high-filling-factor approximation, the dependence on q of the width and peak height of the

envelope is in agreement with the $g=1$ exact energy response as shown in Fig. 1.

We found no structure around $\hbar\omega=2U$ in the exact numerical results. This is consistent with the fact that the parameters used in this paper lie within the regime of validity of first-order perturbation theory.

For the form of energy spectroscopy we consider here, there is no fundamental limit to Bragg pulsed durations, in contrast to momentum spectroscopy.[1] However, practical considerations will likely inhibit the resolution of the individual excitation peaks in current experiments (see discussion below). In this case the envelope shown in Fig. 1 will provide a more realistic depiction of the experimentally observable spectrum.

IV. VALIDITY CONDITIONS

The treatment we present here is based on linear response. In this section we indicate its strict validity conditions in terms of the Bragg strength V_0 which is the relevant experimental parameter.

After the Bragg perturbation is applied, the many-body state is no longer in the BHH ground state $|0\rangle$. The transition probability to an excited state $|i\rangle$, $|c_i(t)|^2$, according to first-order perturbation theory is given by

$$|c_i(t)|^2 = V_0^2 |\langle i|\hat{\rho}_q^\dagger|0\rangle|^2 \frac{\sin^2[(E_i/\hbar-\omega)t/2]}{\hbar^2(E_i/\hbar-\omega)^2}, \tag{10}$$

where the eigenenergies E_i of the states are measured with respect to the ground-state energy. The validity of linear response requires the total excited-state population at the conclusion of the Bragg perturbation to be small compared to unity:

$$\sum_{i\neq 0} |c_i(T_p)|^2 \ll 1. \tag{11}$$

Deep in the Mott regime the response of the system is dominated by the M excited states $|\Phi_i^{(1)}\rangle$. Because all these states have energies $E_i^{(1)}$ approximately given by U, the maximum transfer energy possible is of order U. The validity of linear response constrains the total imparted energy to be much less than U and the heating rate $\delta E/\delta t = U\Sigma_{i\neq 0}|c_i(t)|^2/t$ due to the Bragg perturbation to be much less than U/T_p.

It was previously shown that the M excited states $|\Phi_i^{(1)}\rangle$ have an energy spread given by $4J(2g+1)\cos(qd/2)$ [Eq. (6)], and matrix elements given by $|\langle\Phi_i^{(1)}|\hat{\rho}_q^\dagger|\Phi_0^{(1)}\rangle| \propto J\sin(qd/2)\sqrt{32g(g+1)}/U$ [Eq. (9)]. The average separation between two consecutive states is of order $\Delta E \sim 4J(2g+1)\cos(qd/2)/M$. Individually resolving the different lines will require one to apply the Bragg pulse for a time of order $T_p^{(s)} \gtrsim Mh/[4J(2g+1)\cos(qd/2)]$. The validity of linear response, Eq. (11), therefore requires that

$$V_0 \ll \frac{U}{M}\cot\left(\frac{qd}{2}\right). \tag{12}$$

For the parameters of Ref. [9], where ^{87}Rb atoms are trapped in a lattice of depth $18.5E_R$, the tunneling time h/J is about 0.1 s. The number of occupied wells is $M\sim 20$, with a filling factor $g\sim 1$. Resolving a single peak would require a Bragg pulse of duration $T_p^{(s)}\sim 0.2$ s. With these conditions linear response is valid if $V_0 \ll 0.015\cot(qd/2)E_R$. The acceptable heating rate is much less than $1.8E_R/\mathrm{s}$.

If the duration of the applied perturbation is $T_p \leqslant T_p^{(s)}$, excited states will not be individually discernible. Near resonance ($\hbar\omega\approx U$), for pulse durations smaller than the inverse bandwidth, $T_p < T_p^{(e)}$, $T_p^{(e)} = h/[4J(2g+1)\cos(qd/2)]$, all states will be resonantly excited. If $T_p \sim T_p^{(e)}$ the validity of linear response requires

$$V_0 \ll \frac{U}{\sqrt{M}}\cot\left(\frac{qd}{2}\right), \tag{13}$$

where the factor of $\sqrt{M}$ accounts for the contribution from all M excited states. For the parameters given above this inequality implies $V_0 \ll 0.07\cot(qd/2)E_R$. Here, the acceptable heating rate is much less than $36E_R/\mathrm{s}$.

We note that in the superfluid regime the uncorrelated nature of the system allows for a less stringent validity condition to hold: it is only required that the amount of excited atoms be small compared to the condensate population.

V. FINITE-TEMPERATURE CASE

It is well known in the literature (see for example [17]) that in the superfluid regime, Bragg spectroscopy is not an appropriate tool for probing the temperature of the system. The reason is that even though $S(q,\omega)$ is temperature dependent, experimental observables such as the energy transfer depend on $\chi(q,\omega)$ which is very weakly temperature dependent. This is not the case deep in the Mott-insulator regime. In a translationally invariant lattice all the 1ph excitations have an energy separation of order U from the ground state and a splitting between them of order J. If the temperature is $k_BT \lesssim U/3$, it is still valid to restrict the Hilbert space to the one spanned by the 1ph excitations. In this regime $\chi(q,\omega)$ [see Eq. (4)] can be written as

$$\chi(q,\omega) = \frac{(1-e^{-\beta U})}{\mathcal{Z}}\chi(q,\omega)_{T=0} + \frac{1}{\mathcal{Z}}\chi^{\mathrm{ph}}(q,\omega_{ij}), \tag{14}$$

$$\chi^{\mathrm{ph}}(q,\omega_{ij}) \equiv \sum_{i,j>i} (e^{-\beta E_i^{(1)}} - e^{-\beta E_j^{(1)}})[f_q(\omega_{ij}) - f_{-q}(-\omega_{ij})], \tag{15}$$

where the sum runs over the states in the one-particle-hole band, and $\mathcal{Z}\approx 1+M(M+1)e^{-\beta U}$. The first term in Eq. (14), proportional to $\chi_q(\omega)|_{T=0}$, causes a thermal reduction of the zero-temperature response. The second term, which scales as

[1] Momentum spectroscopy requires that the pulse length does not exceed a quarter of the period of the magnetic trap used to experimentally confine the atoms [11].

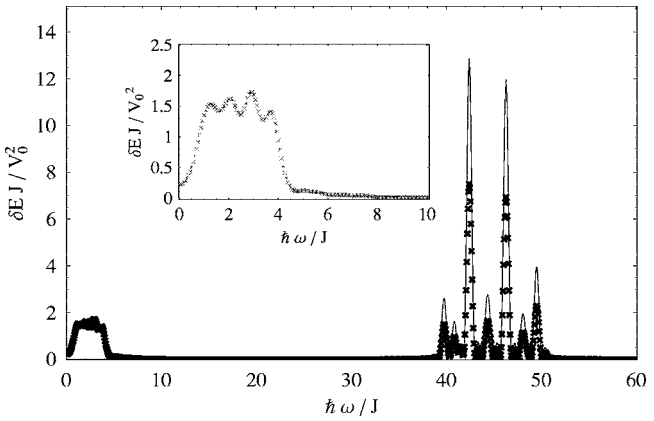

FIG. 2. Energy transfer for a system at finite temperature. Solid line, $k_BT/U=0.007$; crosses, $k_BT/U=0.21$. The other parameters are the same as those in Fig. 1.

$e^{-\beta U}\beta J/\mathcal{Z}$,[2] makes the system sensitive to low-energy Bragg perturbations at frequencies resonant with the energy difference between two 1-ph excitations. The factor $e^{-\beta U}$ suppresses the observability of these thermal effects for $k_BT < U/5$.

In Fig. 2 we plot the energy transfer as a function of the Bragg frequency, as calculated from exact diagonalization of the BHH for two different temperatures. The figure shows that for temperatures $k_BT/U \gtrsim 1/5$ the height of the zero-temperature peaks around U decreases, while low-frequency peaks appear. The presence of these low-frequency peaks is therefore a signature of finite temperature. In particular, if peaks around U are observed in the absence of low-frequency response, the temperature is lower than $U/(5k_B)$. While this analysis does not provide a precise determination of the temperature, it is still useful because it shows that Bragg spectroscopy is sensitive to temperatures of order of the interaction energy. Current experimental techniques do not provide any information on the scale of U. In fact, in current experiments temperature measurements rely on the analysis of atomic interference patterns after a certain time of flight following the release of atoms, and the measurement precision is of the order of the energy spacing to the second lattice band, which is typically one order of magnitude larger than U.

[2]Notice that due to the the zeroth-order degeneracy of the 1ph subspace, $|\langle i|\hat{\rho}_q|j\rangle|^2 \sim 1$.

VI. FINAL REMARKS

In recent experiments [13], Bragg spectroscopy was performed using a setup where the Bragg momentum equals the lattice momentum and the response was observed. Our present analysis, in agreement with previous ones [10,15], predicts no response for $q=2\pi/d$. Using similar perturbative techniques as the ones described here, we extended our calculation to inhomogeneous systems with a strong harmonic magnetic confinement. We also found no scattering for $q=2\pi/d$ in these systems. The fact that neither the inhomogeneity nor the finite size of the system is responsible for the observed signal suggests that nonlinear effects are the most plausible explanation for the experimental results.

In summary, we have shown that Bragg spectroscopy can be a suitable experimental tool for characterizing the Mott-insulator phase. By measuring the transfer energy at different Bragg momenta we proved it is possible to get information about the excitation spectrum: Bragg peaks are centered around the characteristic Mott excitation gap and are contained in an interval whose width is proportional to the 1ph excitation band width. Their average height is maximized when the Bragg momentum approaches π/d. Finally, looking at the low-frequency response we showed that Bragg spectroscopy is sensitive to temperatures of order of the Mott gap.

ACKNOWLEDGMENTS

This work was supported by an Advanced Research and Development Activity (ARDA) contract and by the U.S. National Science Foundation under Grant No. PHY-0100767.

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