Raman spectroscopy of Mott insulator states in optical lattices

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Abstract. We propose and analyse a Raman spectroscopy technique for probing the properties of quantum degenerate bosons in the ground band of an optical lattice. Our formalism describes excitations to higher vibrational bands and is valid for deep lattices where a tight-binding approach can be applied to describe the initial state of the system. In sufficiently deep lattices, localized states in higher vibrational bands play an important role in the system response, and shifts in resonant frequency of excitation are sensitive to the number of particles per site. We present numerical results of this formalism applied to the case of a uniform lattice deep in the Mott insulator regime.

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1. Introduction

The observation of the Mott insulator state of a degenerate Bose gas in an optical lattice [1] has opened an exciting new avenue for investigating strongly correlated condensed matter systems. Ensuing experiments (e.g. [2]–[4]) have investigated a wide variety of phenomena making optical lattices one of the leading systems for studying quantum atom optics.

In the initial experimental report, two key pieces of evidence were given for the Mott insulator state: the loss of phase coherence and the appearance of a gap in the excitation spectrum. More recent experimental work has used Bragg spectroscopy [5, 6] to study the equilibrium properties of this system. While this type of probing reveals the appearance of a gap in the excitation spectrum, experimental applications of this technique operate well beyond the linear response regime, making direct comparison with theory difficult.1

In this paper, we propose and theoretically analyse a Raman spectroscopy scheme for probing Mott insulator states in the lattice system. The formalism we present is sufficiently general to include the excitation of atoms to higher vibrational bands where they should be easily discernible from the unscattered atoms in time-of-flight analysis. We apply this formalism to a uniform lattice and show how the correlated nature of the Mott insulator state can give rise to localized states in the excited bands when the lattice is sufficiently deep, and that the resonant frequency of these localized states is sensitive to the local filling factor in the optical lattice.

2. Formalism

The system of interest, which we will refer to as system 1, is a degenerate collection of bosonic atoms populating the lowest vibrational band of an optical lattice well characterized by the Bose–Hubbard Hamiltonian

\[ \hat{H}_1 = \epsilon_0 \sum_j \hat{n}_j - J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U_{11} \alpha_w}{2} \sum_j \hat{n}_j (\hat{n}_j - 1), \]

where \( \hat{a}_j \) is a bosonic operator that annihilates an atom from the Wannier state \( w_j(x) \) centred on lattice site \( j \), with \( \hat{n}_j = \hat{a}_j^\dagger \hat{a}_j \) the respective number operator. The quantity \( J \), known as the tunnelling matrix element, characterizes the tunnelling between lattice sites and is determined from band structure calculations [7, 8]. Interactions between particles are described by the matrix element \( \alpha_w \equiv \int d^3x |w_j(x)|^4 \) and the coefficient \( U_{11} = 4\pi a_{11} \hbar^2/m \), where \( a_{11} \) is the s-wave scattering length for collisions between atoms in internal state 1. We restrict our attention here to the translationally invariant system (i.e. neglect the influence of external trapping potentials in addition to the optical lattice), and the constant \( \epsilon_0 \) characterizes the mid-point energy of the ground band.

In this work, we consider a scheme for probing the properties of system 1, by an internal state changing Raman transition, of the form used in [9] to output couple an atom laser. A theory for this type of process in an optical lattice has also been proposed by Konabe et al [25].2 This

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1 The observable for Bragg spectroscopy in optical lattices is the energy transferred to the system. This observable is rather difficult to measure accurately, and to obtain a signal experiments necessarily add a large amount of energy, well beyond the linear response limit.

2 We note that the primary difference of our treatment to that of Konabe et al is that we include interactions between scattered and unscattered atoms, which are essential for the main results we present here.
is in contrast to a recent theory [10]–[15] and experiments [5, 6] that have considered internal state-preserving transitions to perform spectroscopy—known as Bragg spectroscopy [16]. A schematic diagram of this coupling is shown in figure 1. Following the formalism in [17], this type of coupling is described by an interaction term of the form

\[
\hat{V} = \frac{V_p}{2} \theta(t) \sum_j \int d^3x \hat{\psi}_2^\dagger(x) \hat{a}_j w_j(x)e^{i(q \cdot x - \omega_0 t)} + \text{H.c.},
\]  

where \(\hat{\psi}_2^\dagger\) is the field operator for bosonic atoms in the second internal state, and the quantities \(\hbar q\) and \(\hbar \omega_0\) specify the momentum and energy transfer of the Raman process respectively. For simplicity, we define \(\hbar \omega_0\) to be the excess energy transferred over the internal state energy difference. We take the amplitude of the Raman coupling to be of strength \(V_p\) beginning at \(t = 0\), and of duration \(T_p\). We will assume that the internal states 1 and 2 are different hyperfine ground states for which we can neglect any collisional spin evolution (see [18, 19]). To arrange such a Raman probe experimentally, a pair of light fields (in addition to those used to create the lattice) with appropriately chosen polarizations to couple the states of interest will need to be applied to the atoms in the lattice. While such a probe could be focused down to address a few sites in a lattice, our theoretical development here is for the case where the Raman fields uniformly illuminate the system and have no spacial selectivity.

Our interest lies in the linear response regime, where only a small portion of the atoms is scattered into internal state 2. The evolution of these atoms in internal state 2, which we will refer to as system 2, is described by the Hamiltonian

\[
\hat{H}_2 = \int d^3x \ \hat{\psi}_2^\dagger(x) \left( H_{sp} + U_{12} \sum j |w_j(x)|^2 \right) \hat{\psi}_2(x),
\]
where

\[ H_{sp} = \left( \frac{p^2}{2m} \right) + V_{ext}(x) \]  

(4)

is the single-particle Hamiltonian with \( V_{ext}(x) \) the external potential (taken to be the same lattice potential experienced by atoms in system 1), and \( U_{12} = 4\pi a_{12}\hbar^2/m \) characterizes the interactions between particles in systems 1 and 2. Within the validity regime of linear response, it is permissible to neglect interactions between atoms in system 2, as their density will remain low.

System 2 is initially in the vacuum state, and the spectroscopic signal to be measured is the number of atoms in system 2 after the Raman pulse. This is a convenient experimental observable as detection techniques can readily distinguish between atoms in different internal states [19]. Additionally, when the coupling produces atoms in an excited vibrational band, the excited atoms can be differentiated by their behaviour upon expansion from the lattice [20, 21]. These properties of the observable should enable the system response to be measured for small amounts of Raman excitation, allowing the system to be probed in the linear response regime.

The expression for the number of excited atoms, derived using linear response theory, is

\[ \langle \hat{N}_2 \rangle = \frac{\pi V_p^2 T_p}{2\hbar^2} \int_{-\infty}^{+\infty} d\omega R(\mathbf{q}, \omega) \frac{2 \sin^2 \left[ (\omega - \omega_0)T_p/2 \right]}{\pi T_p (\omega - \omega_0)^2}, \]  

(5)

where we have introduced the correlation function

\[ R(\mathbf{q}, \omega) = \frac{1}{2\pi} \int dt \int d^3x \int d^3x' e^{i\mathbf{q} \cdot (x' - x) + i\omega t} \sum_{ij} w_i^*(x) w_j(x') \langle \hat{a}_i^\dagger(t) \hat{a}_j(0) \rangle \langle \hat{\psi}_2^\dagger(x, t) \hat{\psi}_2^\dagger(x', 0) \hat{\psi}_2(x') \hat{\psi}_2^\dagger(x, 0) \rangle_{eq}. \]  

(6)

In this expression, the time dependence of the operators is in an interaction picture with respect to unperturbed Hamiltonians \( \hat{H}_1 + \hat{H}_2 \), and the expectation is taken on the initial equilibrium ensemble.

We will now show how to evaluate the correlation function \( R(\mathbf{q}, \omega) \), and how it relates to the properties of the atoms in system 1. We take the initial density matrix to be \( \rho = \rho_1 \otimes \rho_{vac}^2 \), where \( \rho_1 \) is the degenerate lattice state we are interested in probing and \( \rho_{vac}^2 \) is the initial vacuum state for system 2. We can then show that without further approximation, \( R(\mathbf{q}, \omega) \) can be written in the form

\[ R(\mathbf{q}, \omega) = \frac{1}{2\pi} \int dt \int d^3x \int d^3x' e^{i\mathbf{q} \cdot (x' - x) + i\omega t} \sum_{Qij} \langle Q| \hat{a}_i^\dagger(t) \hat{a}_j(0) \rho_1|Q\rangle \langle Q| \hat{\psi}_2^\dagger(x, t) \hat{\psi}_2^\dagger(x', 0) \hat{\psi}_2(x') \hat{\psi}_2^\dagger(x, 0) \rangle_{eq}. \]  

(7)

where the variable \( Q \) represents a trace carried out over the number state basis for the operators \( \{ \hat{a}_j \} \), i.e. \( Q \leftrightarrow |n_{Q-1}, n_{Q}^0, \ldots, 0\rangle \), and \( |0\rangle \) represents the vacuum state of system 2. The operator \( \hat{\psi}_2^\dagger(x, t) \) is \( \hat{\psi}_2(x) \) evaluated in an interaction picture with respect to the Hamiltonian

\[ \hat{H}_j^Q = \int d^3x' \hat{\psi}_2^\dagger(x') \left( H_{sp} + U_{12} \sum_i (n_i^Q - \delta_{ij}) |w_i(x)|^2 \right) \hat{\psi}_2(x). \]  

(8)
We note that in deriving equation (7) we have made use of the result
\[
e^{i\hat{H}_2 t/\hbar} \hat{\psi}_2(\mathbf{x}) e^{-i\hat{H}_2 t/\hbar} \hat{a}_j(0)|Q\rangle = \hat{a}_j(0)|Q\rangle \hat{\psi}_j^Q(\mathbf{x}, t),
\]
and we have made the replacement \(\hat{a}_j(0)|Q\rangle \rightarrow \hat{a}_j(0)|Q\rangle \hat{\psi}_Q j(\mathbf{x}, t),\)
where the \(\delta_{lj}\) term in equation (8) arises from commuting \(\hat{a}_j\) with \(\exp(i\hat{H}_2 t/\hbar)\), and we have made the replacement \(\hat{n}_l \rightarrow \hat{n}_Q j\) as \(|Q\rangle\) are number states.

We refer to \(\hat{H}_j^Q\) as the \(Q\)-defect Hamiltonian for system 2, as it arises from the removal of a system 1 atom from site \(j\) of the number state \(Q\). As the system 1 atoms form an effective potential for those in system 2, the removal of an atom at site \(j\) due to the Raman excitation creates a potential hole (i.e. the \(n_Q j - \delta_{lj}\) term in equation (8)). This defect plays a key role in the response spectrum as we will demonstrate later. Since \(\hat{H}_j^Q\) is a quadratic Hamiltonian it can be diagonalized by numerical methods to obtain its eigenvectors \{\(\phi_{jm}^Q(x)\)\} and eigenvalues \{\(\hbar\omega_{jm}^Q\)\}, i.e. \(\hbar\omega_{jm}^Q \phi_{jm}^Q(x) = \hat{H}_j^Q \phi_{jm}^Q(x)\), where \(m\) is the quantum number specifying the state and \(j\) labels the defect location. We note that in the limit \(U_{12} \rightarrow 0\), the \(\phi_{jm}^Q\) reduce to the Bloch states of \(H_{sp}\) and \(m\) becomes the quasimomentum and band index. We obtain \(\hat{\psi}_j^Q(\mathbf{x}, t) = \sum_m \phi_{jm}^Q(x) \hat{b}_jm e^{-i\omega_{jm}^Q t}\),
where \(\hat{b}_jm\) is a bosonic annihilation operator and arrive at the expression
\[
R(q, \omega) = \frac{1}{2\pi} \int dt e^{i\omega t} \sum_Q \sum_{ijm} c_{ij}^Q(t) A_{mij}^Q A_{mij}^{Q*} e^{-i\omega_{jm}^Q t},
\]
where we have defined
\[
A_{mij}^Q \equiv \int d^3x \phi_{jm}^{Q*}(x) e^{iq \cdot x} u_i(x),
\]
\[
c_{ij}^Q(t) \equiv \langle Q|\hat{a}_i^+(t)\hat{a}_j(0)|Q\rangle.
\]

Equations (7) and (10) represent the key results of this work, and we now briefly comment on the physical process they describe. Fundamentally, \(R(q, \omega)\) characterizes the excitation spectrum of atoms from system 1 into system 2. In the context of ultra-cold gases, a result similar to our starting point (equation (5)) has been given by Luxat and Griffin [22] for the case of a harmonically trapped Bose gas (also see [23, 24]). However, their treatment neglects interactions between atoms in different hyperfine states and assumes that the single-particle correlation functions for the atoms in systems 1 and 2 are independent. The extension of this theory to the optical lattice, has been provided by Konabe et al [25]. For the current experiments with Rubidium atoms in a deep optical lattice, these approximations are not tenable. In particular, as we noted previously, the lattice site from which the atom is excited acts as the localizing defect and accounting for correlations between the systems (as we have done in equation (7)) is essential.

We note that our formalism (i.e. equations (7) and (10)) is quite general. As long as the dominant number states of the many-body state are known, e.g. through exact diagonalization or Matrix Product Decomposition techniques (see e.g. [26]), then the Raman response can be determined. In the following sections, we consider the application of our formalism for two special cases. The results we present in section 3 are calculated for one-dimensional (1D) systems for numerical convenience, though our interest is in the regime where the scattering between particles is 3D and well-described by a contact interaction.
3. Single-site limit

The limiting case of a single tightly confining harmonic well of frequency $\omega_{ho}$ is a useful approximation to a deep lattice in the regime where tunneling between sites can be neglected. This limit shows the main physical features of Raman spectroscopy and provides a useful approximation to the full solution. Assuming that interaction shifts are small compared to the oscillator energy $\bar{\hbar}\omega_{ho}$, we may approximate the modes of the system as being harmonic oscillator eigenstates $\{\varphi_m(x)\}$, with respective energies $\{\epsilon_m = \hbar\omega_{ho}(m + 1/2)\}$. For the single-site case, our formalism maps according to

$$w_j(x) \rightarrow \varphi_0(x),$$

$$\varphi^0_{jm}(x) \rightarrow \varphi_m(x),$$

$$A^0_{mij} \rightarrow A_m = \int d^3x \varphi^*_m(x) e^{i\mathbf{q} \cdot \mathbf{x}} \varphi_0(x),$$

$$\hbar\omega_{jm} \rightarrow \hbar\omega^*_m = \epsilon_m + U_{12}\alpha_{0m}(n - 1),$$

where $\alpha_{0m} \equiv \int d^3x |\varphi_0(x)|^2 |\varphi_m(x)|^2$. Since the Hamiltonian for system 1 reduces to $\hat{H}_1 \rightarrow \epsilon_0\hat{n} + U_{11}\alpha_\nu\hat{n}(\hat{n} - 1)/2$ in this limit, we have replaced $Q$ by $n$ (i.e. the single-site many-body number states are just single mode number states $|n\rangle$ of mode $m$) and evaluated the correlation function as

$$c^0_{ij}(t) \rightarrow c^0_{ij}(t) = n \exp\{i[\epsilon_0 + U_{11}\alpha_\nu(n - 1)]t/\hbar\}. \quad (17)$$

Using equation (10) with $\rho_1 = \sum_{m'n'} |n\rangle \rho_{nn'} \langle n'|$, we obtain

$$R(q, \omega) = \sum_n \rho_{nnn} |A_m|^2 \delta[\omega_{res}(n) - \omega], \quad (18)$$

$$\hbar\omega_{res}(n) = \epsilon_m - \epsilon_0 + (U_{12}\alpha_{0m} - U_{11}\alpha_\nu)(n - 1). \quad (19)$$

We have also assumed that the probe only couples to a particular excited state $m$, with the other states sufficiently far detuned that their contribution is negligible.

Equation (18) shows that the response of the system is proportional to $\rho_{nn}$, and most notably, if $(U_{12}\alpha_{0m} - U_{11}\alpha_\nu) \neq 0$, then the response frequency is linearly dependent on the value of $n$ (i.e. the number of atoms at the site). In this regime, the Raman spectrum reveals the number distribution at the site. For the case of $^{87}$Rb (the atom of primary interest in bosonic optical lattice experiments), the interactions between the relevant hyperfine states are approximately degenerate (i.e. $U_{11} \approx U_{12}$), so that the difference $\alpha_{0m} - \alpha_\nu$ will be the primary factor in determining the magnitude of the number-dependent shift. As an immediate consequence, we note that for the case $U_{11} = U_{12}$ and a Raman pulse coupling to ground vibrational state of system 2, the spectrum will be independent of $n$ (i.e. for $m = 0$ we have $\alpha_{0m} = \alpha_\nu$). Therefore to obtain a number-dependent spectral response with $^{87}$Rb will require scattering into excited vibrational states of system 2.
4. Uniform Mott insulator

We now consider the more general case of a translationally invariant lattice with \( N_s \) sites and periodic boundary conditions. We assume that the number of atoms in the system is commensurate with the number of lattice sites and system is deep in the Mott insulating regime, where \( U_{11} \alpha_w \gg J \). In this regime, the many-body ground state is well approximated as \( |Q_n\rangle = |..., n, n, ...\rangle \) (i.e. a definite number of atoms at each site). In calculating the response of the system to the Raman probe according to equation (7), the summation over \( Q \) reduces to this single state. The next order correction to the translationally Mott state is particle hole states \([13]\), which contribute to the ground state with an amplitude \( J/U_{11} \alpha_w \ll 1 \), and can be neglected.

To obtain an approximation for the temporal correlation function of system 1 in state \( |Q_n\rangle \), we ignore the tunnelling term in \( \hat{H}_1 \). This approximation amounts to neglecting particle tunnelling between sites in system 1 over the timescale of the Raman probe, and should be a good approximation in deep lattices. In this limit, the correlation function is

\[
c_{ij}^{Q_n}(t) = n \exp\{i[\epsilon_0 + U_{11} \alpha_w(n - 1)]t/\hbar\}\delta_{ij},
\]

and making use of the translational invariance in evaluating equation (10) we obtain

\[
R(\mathbf{q}, \omega) = \sum_m n N_s |A_{ml}^{Q_n}|^2 \delta(\omega - \omega_{\text{res}}^{Q_m}),
\]

\[
\omega_{\text{res}}^{Q_m} = \omega_{lm}^{Q_n} - [\epsilon_0 + U_{11} \alpha_w(n - 1)]/\hbar.
\]

Note that due to translational invariance the precise value of \( l \) used in equation (17) is unimportant. We now calculate the response spectrum \( \langle \hat{N}_2 \rangle \) using equations (5) and (17) for a translationally invariant 1D lattice. We take the lattice potential to be \( V_{\text{ext}}(x) = V_D \cos^2(x/\lambda) \), arising from counter-propagating laser fields of wavelength \( \lambda \), and we specify the lattice depth \( V_D \) in units of \( E_R = h^2/2m\lambda^2 \). The calculation is performed for typical \(^{87}\)Rb parameters (see e.g. [1]) to demonstrate the practicality of our probing scheme. We will not consider the influence of \( \mathbf{q} \) on the spectrum in this paper,\(^3\) and for simplicity we have taken \( \mathbf{q} \) as being identical to a reciprocal lattice for our calculations.

The results we have obtained are shown in figure 2. For the case of \( V_D = 10E_R \) (figure 2(a)), the Raman response is shown over a frequency range that includes resonant coupling to the first two excited bands. The superimposed graphs show the spectra for Mott insulating states of various filling factors and clearly exhibit frequency shifts proportional to \( n \). Additionally, we notice that in the first excited band (12–18 kHz), the dominant response peak occurs at the low end of the spectral feature (e.g. the peak at \( \sim 15.5 \) kHz for \( n = 1 \)), adjacent to a broad base. This feature is also seen in the 2nd excited band (24–36 kHz), however the peaked feature is much less dominant relative to the broad base. The peak originates from an excited band state that is partially localized above the defect site. This localization leads to a strong coupling matrix element \( A_{ml}^{Q_n} \), and as this state resides at the defect, its energy is lower than the other states in the excited band. We refer to this state as the defect state, which is clearly identified as the most strongly excited feature at the bottom of each spectral band. Since the localization is not perfect,

\(^3\) Generally, large \( q \) favours coupling to higher bands, though certain choices of \( q \) can suppress coupling efficiency, e.g. for \( q = 0 \) the response from the first excited band is zero by symmetry.
Figure 2. The percentage of atoms excited after Raman excitation in a 1D lattice of depth (a) $V_D = 10E_R$ and (b) $V_D = 30E_R$. In each plot, the spectrum of Mott insulator states with filling factors of $n = 1$ (dark line), $n = 2$ (medium line) and $n = 3$ (light line) are shown. The respective single-site results for $m = 1$ are given as dashed lines. Parameters are $q = \pi/\lambda$, $T_p = 1.5\,\text{ms}$, $V_p = 0.05E_R$, $\lambda = 850\,\text{nm}$, $N_s = 51$, transverse confinement taken to be harmonic with $f_\perp \approx 37.6\,\text{kHz}$, and $a_{11} = a_{12} = 5.29\,\text{nm}$.

the other states in the excited band have appreciable amplitude at the defect site. These states give rise to the broad, though more weakly excited, band of states above the resonant peak. In the 2nd excited band, the same features are seen, however, as the effective tunnelling in this band is much higher, and the defect state is much less localized.

In figure 2(b), the response spectrum is shown for a lattice of depth $V_D = 30E_R$. At this depth, the response from the first excited band states have shifted up to 30 kHz, and the second excited band has moved out of the frequency range considered. In contrast to the spectrum in figure 2(a), we only notice the resonant peak due to the defect state, without a discernible broad base of band states. This arises because at this depth the tunnelling rate in the excited band is sufficiently small that the defect state becomes completely localized. The other states in the excited band are necessarily orthogonal to the defect state and so have vanishing coupling matrix elements $A_{mll}$.

For comparison, in figures 2(a) and (b), we also show the single-site predictions for the spectrum calculated using expression (18) with $\omega_{ho}$ chosen to match the effective trap frequency at the lattice site minima. The frequency location of the response spectra compares badly with the full lattice solution, arising primarily from the inadequacy of the harmonic approximation for accurately predicting band structure. The location of the spectra can be easily corrected for by calculating the term $\epsilon_m - \epsilon_0$ in the expression for $\omega_{res}(n)$ using the non-interacting band structure result. However, the single-site approximation captures many of the salient features of the full lattice solution, such as the magnitude of the $n$-dependent shift in the response spectrum. In the strongly localized defect limit (figure 2(b)), the single-site approximation quantitatively predicts the response amplitude as the role of the band states can be neglected.
To quantify the emergence of the defect state, we examine the spectrum of $\omega^{Qnm}_{\text{res}}$ as a function of $V_D$ in figure 3(a). For $V_D \gtrsim 13.5 E_R$, a single defect state is observed to drop below the first excited band. The condition for the emergence of a strongly localized defect state is that the energy reduction from localization above the defect in system 1 is large compared to the effective inter-site tunnelling in the excited band. To verify this criterion, we compare the excited bandwidth (characterizing the excited band tunnelling rate) and energy reduction at the defect, approximated by $U_{11} \alpha w$. These two energy scales are seen to cross at $V_D \approx 13.5 E_R$. Finally, we note the validity condition for linear response treatment of Raman spectroscopy. This requires the number of atoms excited to remain small compared to the total number of atoms in the system. In terms of the Raman parameters, this condition is given as $n V_p^2 T_p^2 / 4 \hbar^2 \ll 1$, where $n$ is the average number of atoms per site.

We briefly comment on the relationship of the 1D calculations presented here to an equivalent system in a 3D lattice. The primary difference in applying our formalism to a fully 3D system is that equation (8) will need to be solved in 3D. For the case of coupling to excited bands, the tunnelling between lattice sites can occur in all directions, but is dominated along the direction in which the vibrational excitation has occurred. This direction will be parallel to the direction of the momentum transfer in the Raman coupling, which we take to be parallel to a lattice vector. The tunnelling in the orthogonal directions will be given by the ground band tunnelling rate which is typically much smaller. This suggests that the additional shifts in a fully 3D lattice will be of order of the ground state tunnelling rate and will thus contribute small corrections to the results presented here. A full study in 3D will be the subject of a future investigation.

5. Conclusions and outlook

In this work, we have proposed and analysed a Raman spectroscopy technique for probing the properties of quantum degenerate bosons in the ground band of an optical lattice. We have
observed that for sufficiently deep lattices, localized states in higher vibrational bands play an important role in the system response, and shifts in resonant frequency of excitation are sensitive to the number of particles per site. While our main study has considered the case of a perfect Mott insulator in a translationally invariant lattice, our results suggest that in the limit of strongly localized defect states the response of the system is well-described by the single-site result, and thus only depends on the local number distribution at each lattice site. The Raman spectrum may therefore be a useful method for measuring the relative portion of system 1 at sites with filling factor $n$ atoms. We speculate that in the strongly localized limit, the homogeneity of the lattice is rather unimportant, and the existence of the defect states arises from the large difference in the effective potential energy between the site where the particle is excited and the neighbouring site. This suggests that many of the predictions we have made here, and in particular the results of the one-site model, should qualitatively apply to inhomogeneous lattices, such as the combined harmonic and optical lattice potentials made in experiments. In this case, as well as in the superfluid limit (where significant number of fluctuations exist), significant corrections may arise from resonances between neighbouring sites that would allow the defect state to be delocalized over several sites. However, it seems reasonable to expect that these resonances would contribute to the broad background in the Raman spectrum, and the sharp features from Mott insulating regions (if present) would be clearly visible. Characterizing the role of superfluid fluctuations and the external confining potential will be the subject of future work.

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Note added in proof. An experimental report presenting results in agreement with our theory has recently appeared [27]. In that paper microwave and RF fields were used to arrange a Raman coupling with $q \approx 0$, allowing transitions to another hyperfine state, but restricted to the ground band. In this limit the resonant frequencies are only sensitive to the small scattering length differences, often referred to as the clock shift. Our theory describes this case, for instance equation (19) reduces to

$$\omega_{\text{res}} = \frac{(U_{12} - U_{11})\alpha_w(n - 1)/\hbar}{\sqrt{\hbar}}$$

in this limit, in agreement with the experimental results.

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