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Matter-Wave Scattering from Ultracold Atoms in an Optical Lattice

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We study matter-wave scattering from an ultracold, many-body atomic system trapped in an optical lattice. The angular cross section of the target lattice for a matter wave is determined and is demonstrated to have a strong dependence on the many-body phase, superfluid, or Mott insulator. Analytical approaches are employed deep in the superfluid and Mott-insulator regimes, while intermediate points in the phase transition are treated numerically. Matter-wave scattering offers a convenient method for nondestructively probing the quantum many-body phase transition of atoms in an optical lattice.

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Ultracold atoms in an optical lattice form an optical crystal that permits the clean implementation of fundamental models of condensed matter physics to a degree unheard of in other systems. The physical parameters characterizing this system, the depth of the lattice, and the interactions of the atoms in the lattice, are experimentally tunable so that it is possible to probe the atoms’ behavior controllably from noninteracting single particle mechanics to strongly interacting, many-body physics [1–3]. Of particular interest are the many-body theories of quantum phase transitions [4], whose predictions can be observed in such a system.

The superfluid to Mott-insulator phase transition has been probed experimentally by studying the interference of clouds of atoms expanding freely out of an optical lattice [5]. This method reveals correlation properties of the ground state of the cold atom system, but does not depend on the excitation spectrum of the lattice, which is essential to study the superfluid fraction [6,7]. Bragg spectroscopy has been combined with this method in order to examine the excitation spectrum [8,9]; nevertheless, it requires the destruction of the sample under examination. Recent, non-destructive theoretical proposals indicate that properties of the ground state, such as on-site number statistics, may be accessible by observing light scattered in an optical cavity [10]. The effect of the many-body phase on the scattering cross section of cold atoms in a lattice for photons has also recently been theoretically examined [11]. Polarization spectroscopy with light for ultracold spinor gases has been explored as a means of probing magnetic ordering [12]. Very little attention has been paid to the interaction of matter waves with these optical crystals. Theoretical work exists examining the impact of disordered atoms in a periodic potential on scattering of photons and particles [13]. We are interested, however, in the impact of the many-body phase on matter-wave scattering.

The scattering of matter waves from a lattice system provides a very useful technique to probe the many-body phase transition both because it does not require the destruction of the lattice under examination and because it depends strongly on the excitation spectrum of the target. This is critical to probe superfluidity and the dynamics of the lattice, beyond analysis of ground state properties. In addition, the simpler form of the interaction, compared with light, between a slow moving probe atom and the atoms in the lattice emphasizes structure that depends only on the many-body properties of the lattice. As we will show, the differential cross section is a highly suitable quantity for the distinction between the Mott-insulating and superfluid phases. As the many-body phase transition occurs, and the energy spectrum of the target is transformed, the behavior of the inelastic cross section qualitatively changes and indicates the presence of a superfluid fraction.

Our objective has been to study the scattering patterns of matter waves due to passage through ultracold atoms trapped in an optical lattice. The scattering target is well modeled by the Bose-Hubbard Hamiltonian, \( \hat{H}_{\text{BH}} \) [1],

\[
\hat{H}_{\text{BH}} = -J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{a}_{\mathbf{r}} \hat{a}_{\mathbf{r}'} + \frac{1}{2} U \sum_{\mathbf{r}} \hat{n}_{\mathbf{r}} (\hat{n}_{\mathbf{r}} - 1).
\]

The probe is a free particle of mass \( m \) with Hamiltonian, \( \hat{H}_p = \hat{p}^2 / 2m \), which does not interact with the confining light of the lattice. We employ low energy probes that avoid interband excitations of atoms in the lattice. In this case, \( s \)-wave scattering is dominant, and we may treat the interaction between the probe and each lattice atom as a pseudopotential with scattering length \( a_s \). The total interaction potential is \( \hat{V} = \sum_j \frac{2m a_s}{\hbar^2} \delta (\hat{\mathbf{r}} - \hat{\mathbf{r}}_j) \) [14]. The operators \( \hat{\mathbf{r}} \) and \( \hat{\mathbf{r}}_j \) give the positions of the probe and the \( j \)th lattice atom, respectively. The full Hamiltonian for the scattering interaction is \( \hat{H} = \hat{H}_p + \hat{H}_{\text{BH}} + \hat{V} \).

Before and after scattering of the probe, the target is in a many-body state of the \( N \) atoms in the lattice. The ground state of the lattice depends on the relative sizes of the interaction strength \( U \) and the tunneling matrix element \( J \), appearing in the Bose-Hubbard model. For weak repul-
sion, the atoms in the lattice will delocalize and the superfluid fraction will increase to one as the interaction strength goes to zero [7]. As the repulsion becomes large compared to the tunneling matrix element, the atoms will localize, the superfluid fraction will go to zero, and a gap will open in the excitation spectrum, giving rise to the Mott-insulator state.

It is possible to alter the interaction strength between the atoms in the lattice by adjusting the depth of the lattice, or by manipulating the scattering length of lattice atom collisions through a Feshbach resonance. Changing the lattice depth, however, affects the density profile of the atoms in the lattice. In order to eliminate consequent effects on the scattering cross sections, it is more desirable to retain a constant lattice depth and employ a Feshbach resonance to alter the interaction strength between the lattice atoms.

The probe is initially a plane wave $|k_0\rangle$ that collides with a target in the ground state $|n_0\rangle$ of the Bose-Hubbard Hamiltonian, with energy $E_{n_0}$. The collision results in a transfer of momentum, $\mathbf{k} = k_0 - \mathbf{k}$, from the probe to the target. Consequently, the target is left in a potentially excited final state $|n\rangle$. The energy lost by the probe is transferred to the lattice atoms so that $E_n - E_{n_0} = \frac{\hbar^2}{2m}(k_0^2 - k^2)$. In the first Born approximation, the scattering cross section separates into two factors, one of which is determined by the binary interaction between the probe and each individual atom in the many-body target. The other is determined solely by the structure of the target [15]. This is true for general choices of the interaction potential. In the case of the pseudopotential, the scattered wave from an individual atom in the target is a structureless spherical wave, and the total angular cross section is given by

$$
\frac{d\sigma}{d\Omega} = a_s^2 \sum_n \sqrt{1 - \frac{E_n - E_{n_0}}{\frac{\hbar^2}{2m}(k_0^2 - k^2)}}, \langle n | \sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{r}_j} | n_0 \rangle \rangle^2. \quad (2)
$$

The matrix element of the momentum boost gives the transition amplitude between the ground and excited states of the target due to a transfer of momentum $\mathbf{k}$ from the probe. The term under the square root, which is the ratio of the outgoing to the incoming probe wave number, diminishes the weight of scattering channels at progressively higher energy. The radicand must be greater than zero, due to energy conservation. The outgoing probe wave number $k$ is determined by the transfer of energy to the lattice and depends on the index $n$ of the final state. The cross section depends only on the angle between the outgoing wave vector $\mathbf{k}$ and the incident wave vector $\mathbf{k}_0$. A natural choice of units for the cross section is the square of the scattering length $a_s$. The cross section in Eq. (2) accommodates the possibility of an external trap; however, in order to isolate the effect of the many-body phase, we specify to the case in which the probe matter wave is focused on a homogeneous phase region. For very strong or very weak repulsion between the atoms in the lattice, it is possible to evaluate the cross section in Eq. (2) analytically. At intermediate values of $U/J$, we do so by numerically diagonalizing the target Hamiltonian.

For very weak interactions, we treat the target as a condensate of $N$ atoms in the ground state of a lattice with $N_L$ sites. Collisions with the probe can elevate atoms out of the condensate into higher energy Bloch modes. These channels contribute to the cross section through the matrix elements of the momentum boost in Eq. (2). This quantity is readily evaluated and understood as the Fourier transform of matrix elements of the density, $\langle n | \hat{\rho}(r) | n_0 \rangle \rangle$. The expression vanishes if more than one atom is scattered out of the condensate. When a single atom is excited into a mode, $\psi_q(r)$, with quasimomentum, $q \neq 0$, we find that $\langle n | \hat{\rho}(r) | n_0 \rangle \rangle = \frac{N}{N_L} |\psi_0(r)|^2$. Exciting a single atom raises the energy of the target by the difference between the energies of the single particle Bloch modes, so that $E_n - E_{n_0} = \epsilon(q) - \epsilon(0)$, where $\epsilon(q)$ is the energy of the specified mode. The diagonal matrix element, which corresponds to elastic scattering, must be handled separately, and is given by $\langle n_0 | \hat{\rho}(r) | n_0 \rangle \rangle = \frac{N}{N_L} |\psi_0(r)|^2$. The additional factor of $\sqrt{N}$ differentiates the scale of the elastic and inelastic cross section and can be traced to the coherent overlap of waves scattered elastically from individual sites.

These results permit us to construct a very general expression for the cross section of the superfluid ground state for a matter-wave incident at any angle upon the optical lattice,

$$
\frac{1}{a_s^2} \frac{d\sigma}{d\Omega} = N(N - 1) \int d^3 r e^{i\mathbf{k}\cdot\mathbf{r}} |\psi_0(r)|^2 \frac{N_L}{1 + N \sum_q \sqrt{1 - \frac{\epsilon(q) - \epsilon(0)}{\frac{\hbar^2}{2m}(k_0^2 - k^2)}} \left| \int d^3 r e^{i\mathbf{k}\cdot\mathbf{r}} |\psi_q(r)|^2 \frac{N_L}{N} \right|^2}. \quad (3)
$$

The elastic cross section is the $q = 0$ component of Eq. (3). Waves scattered elastically from individual lattice sites overlap coherently and lead to Bragg peaks, the scale of which can be determined from the height of the central peak, $\frac{1}{a_s^2} \frac{d\sigma}{d\Omega}(\mathbf{k} = 0) = N^2$. The Fourier transform in the first term has peaks at reciprocal lattice vectors that become increasingly sharp as the number of lattice sites increases. The sum over Bloch modes with $q \neq 0$ in the second term is the inelastic cross section. Including $q = 0$ in the sum gives exactly $N$ times the cross section of a single atom in the lattice and is due to scattering incoherently from each of the $N$ atoms in the target.

We can estimate the scale of this term when the energy transfer from the probe is negligible compared to its initial energy. A typical lattice depth is $V_0 = 15 E_r$, in units of the recoil energy, $E_r = \frac{\hbar^2 k_0^2}{2m_r}$, for photons with wave number $k_0$ and lattice atoms of mass $m_r$. At this depth, the width of the lowest band is $0.03 E_r$ and the band gap
between the first and second bands is \(6.28E_r\), so it is readily possible to have probe energies much larger than the lowest band width, but too small to cause interband excitations. Under these conditions, the initial and final wave numbers of the probe are approximately equal, so that the second term in Eq. (3) simplifies to the number of atoms in the lattice, \(N\).

There are two major features to the scattering from a superfluid: narrow elastic Bragg peaks that scale as \(N^2\) and a superimposed inelastic background that scales as \(N\). The Bragg peaks, as we will demonstrate when we consider the Mott-insulator cross section, are located at positions where the momentum transfer \(\kappa\) is a reciprocal lattice vector. The general expression for the superfluid cross section given in Eq. (3) is shown in Fig. 1 for the specific case of a one-dimensional lattice arranged perpendicular to the incident probe wave vector. As the number of lattice sites increases, the width of the elastic peaks will become increasingly narrow. Away from the peaks, the inelastic background is readily identifiable. This background emerges due to the availability of excited state modes to the condensate. The scattering behavior is qualitatively different when the interaction strength between atoms in the lattice becomes very large.

As the atoms in the lattice repel each other more strongly \((U/J \rightarrow \infty)\), the superfluid fraction decreases, and the atoms become localized within individual wells of the lattice. In this regime, the atoms are no longer found in spatially extended Bloch waves. For a sufficiently strong interaction and commensurate filling, the Mott-insulator state forms, and the ground state of the target can be represented by the number of atoms at each lattice site, \(\tilde{n} = N/N_L\), where \(\tilde{n}\) is an integer. As before, the cross section depends on the state of the target through matrix elements of the density, \(\langle n|\tilde{n}(r)|n_0\rangle\). The expansion of the density operator in a Wannier basis, using the Wannier function for the lowest band of the lattice, \(w(r)\), leads to the interpretation of the matrix element as the amplitude for displacing a single atom from its initial position in the lattice. In terms of on-site field operators, the density operator is \(\hat{n}(r) = \sum_{\mathbf{R},\mathbf{R}'} w^{\dagger}(\mathbf{r} - \mathbf{R}_{\mathbf{k}})w(\mathbf{r} - \mathbf{R}_{\mathbf{k}}')\hat{a}_{\mathbf{R}}\hat{a}_{\mathbf{R}'}\). The \(R_1 = R_2\) terms are elastic channels in which the state of the target is unchanged, \(\langle n|\tilde{n}(r)|n_0\rangle\). Inelastic scattering corresponds to \(R_1 \neq R_2\). The general result for the amplitude to shift a target atom from a site at \(\mathbf{R}\) to \(\mathbf{R}'\) is proportional to the product of the Wannier functions at each site, \(\langle n|\tilde{n}(r)|n_0\rangle = \sqrt{(\tilde{n} + 1)\tilde{n}}w^{\dagger}(\mathbf{r} - \mathbf{R})w(\mathbf{r} - \mathbf{R}')\). Using this expression, we may already anticipate for deep lattices the lesser role inelastic scattering will play due to the weak overlap between atoms at different lattice sites. The energy cost associated with displacing one atom from the uniform ground state is the interaction strength \(U\), which is also the size of the Mott-insulator gap. These results allow us to construct the general expression for the scattering cross section of the Mott-insulator target,

\[
\frac{1}{a_s^2} \frac{d \sigma}{d \Omega} = \tilde{n}^2 \left| \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \right|^2 \times \left| \int d^3r e^{i\mathbf{k} \cdot \mathbf{R}} |w(r)|^2 \right|^2 + \tilde{n}(\tilde{n} + 1)W \sum_{\mathbf{R} \neq \mathbf{R}'} \left| \int d^3r e^{i\mathbf{k} \cdot \mathbf{R}} w^{\dagger}(\mathbf{r} - \mathbf{R})w(\mathbf{r} - \mathbf{R}') \right|^2 ,
\]

with \(W = \sqrt{1 - U/(\hbar^2k_0^2/2m)}\). The sum over the finite number of lattice sites in the first term has a maximum when the momentum transferred from the probe is a reciprocal lattice vector, with \(\mathbf{k} \cdot \mathbf{R}\) an integer multiple of \(2\pi\).

As the number of lattice sites increases, these elastic Bragg peaks narrow, approaching delta functions for an infinite lattice. The central peak has a height, \(\frac{1}{a_s^2} \frac{d \sigma}{d \Omega} (\mathbf{k} = 0) = N^2\). In addition, there is an approximately Gaussian envelope due to the Fourier transform of the Wannier function.

The elastic cross sections of the Mott insulator and superfluid overlap significantly and scale as \(N^2\); however, inelastic scattering from the Mott insulator is strongly suppressed (see Fig. 1). If the incident energy of the probe is less than the energy gap \(U\), the inelastic scattering vanishes completely. Even for probe energies exceeding the gap, the integral in the inelastic part of the cross section in Eq. (4) is negligible under tight binding conditions, so that we expect only elastic scattering.

We can estimate the scale of the Mott insulator’s inelastic background more precisely by using the harmonic approximation of the Wannier function. Near to the central peak, the inelastic background decays exponentially with the lattice strength as \(\exp[-\frac{\pi^2}{2} \sqrt{\frac{6}{E_r}}(j - l)^2]\), where \(j\) and \(l\)
scattering, as a function of \( \theta \), which is the nearest minimum in the elastic peak to forward scattering. The inset shows the numerical cross section at the vertical dashed line, which is the nearest minimum in the elastic peak to forward scattering, as a function of \( U/J \).

FIG. 2 (color online). Cross sections for a probe with energy \( \epsilon = 1E_r \), a lattice depth, \( V_0 = 15E_r \), with 4 atoms and 4 sites, and \( J = 0.0047E_r \). At this energy, the maximum transfer of momentum to the lattice is smaller than the first reciprocal lattice vector, so that only the central peak is visible. The next peak appears for probe energy greater than \( 4E_r \). The values of \( U/J \) shown are 0, 4, 8, and 16. The superfluid analytic result (light gray) for the inelastic background scales as \( N \). The corresponding background for the Mott insulator (dark gray) is strongly suppressed. The inset shows the numerical cross section at the vertical dashed line, which is the nearest minimum in the elastic peak to forward scattering, as a function of \( U/J \).

\((j \neq l)\) are positions of lattice sites in units of lattice spacings. For typical lattice depths, the inelastic contribution is strongly suppressed at all probe energies. This contrasts markedly with the superfluid cross section, which carries a prominent inelastic background that scales as the number of atoms in the lattice. In the regions between the Bragg peaks, this background unambiguously indicates the many-body phase.

We have also examined the disappearance of the inelastic background as the interaction strength \( U/J \) increases from zero. We evaluate the cross section in Eq. (2) at intermediate values of \( U/J \) by exactly diagonalizing the Bose-Hubbard Hamiltonian for small lattices (see Fig. 2). At \( U/J = 0 \), the numerical result coincides with the analytic result for the pure superfluid, and an inelastic background proportional to \( N \) is apparent. This background decays to zero as the interaction strength increases, and the cross section converges on the analytic result we gave for the Mott insulator. The amplitude of the inelastic background has decayed by more than half at \( U/J = 8 \), and it is largely gone for \( U/J = 12 \). This coincides with the range over which the superfluid fraction vanishes [7]. The emergence of a gapped target spectrum corresponds to elimination of the inelastic background. This suggests an increasing sharpness in the decay of the inelastic background for increasing system sizes.

Our analytic results for the scattering cross section in the weakly and strongly interacting regimes show that the many-body phase in the lattice strongly affects the scattering cross section of a low energy matter-wave probe. The periodic nature of the target gives rise in both many-body phases to coherent Bragg peaks whose height scales as the square of the number of atoms in the lattice. In addition, an inelastic background, determined by the excitation spectrum of the target, indicates the presence of superfluidity and scales as the number of atoms in the target. This provides an easily identifiable signature of the many-body phase.

Matter waves offer an effective method for nondestructively probing the many-body phase in an optical lattice. More broadly, the scattering of matter waves depends strongly on properties such as the distribution of atoms in a partially filled lattice, and on the long range correlations and other manifestly quantum mechanical effects found in this novel state of matter. This makes this technique well suited for examining a range of phenomena, including the effect of inhomogeneity of bosons and fermions and disorder in the lattice, in addition to probing the many-body quantum phase transition.

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