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Bragg Diffraction in an Atomic Lattice Bound by Light

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We observe Bragg diffraction of blue (422 nm) radiation from ultracold rubidium atoms bound in an infrared (780 nm) optical lattice thus demonstrating the long range periodic order in these atomic lattices. The blue light is reflected from the [201] planes of a cubic body-centered lattice at an incidence angle of 57° . The angular breadth of the Bragg resonance is limited by the size of the atomic lattice to less than 0.26 mrad. We use Bragg diffraction in combination with an additional weak infrared probe beam as a novel tool to selectively study the motion of atoms deeply bound in the potential wells.

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Optical lattices are three-dimensional periodic arrays of ultracold atoms bound in micropotentials induced by the ac Stark effect in standing light waves. This novel state of matter was first demonstrated a few years ago and has received much attention since [1]. Adjacent lattice sites are separated by several hundred nanometers, while atoms bound inside the potential wells are localized to only a fraction of an optical wavelength. The quantization of the atomic center-of-mass motion gives rise to nearly equidistant energy levels. This discrete energy structure has been observed with spectroscopic methods in various experiments which provided information on the vibrational temperature (700 nK have recently been achieved [2]) and on the degree of atomic localization [3]. However, up to now there has been no way to experimentally obtain direct structural information about the long range order in optical lattices.

This limitation has inspired research on the possibility of Bragg diffraction in optical lattices analogous to the case of crystalline solids for which this method dates back to the famous experiment by Laue, Knipping, and Friedrich in the beginning of this century. Bragg diffraction represents the appropriate technique to investigate all kinds of density correlations such as long range periodic order, deviations from an average lattice, or dynamic collective properties [4]. One may wonder whether the low filling factor in presently realized optical lattices (typically 5% of the available lattice sites are occupied) prohibits the observation of Bragg diffraction, as one would expect in condensed matter samples. But in contrast to crystals where empty lattice sites cause strong perturbations of the periodicity, the long range order in sparsely populated optical lattices should be preserved over the entire extension of the light field. On the other hand, the lattice geometry can be distorted at higher densities which might be reached by novel kinds of optical lattices [5]. These distortions can result from the back action of the induced atomic polarization which modifies the structure of the lattice field [6,7], or from mutual atomic interactions which modify the shape of the potential wells and

may even lead to deviations from a random density distribution [8]. Bragg diffraction would provide access to these effects which are of particular interest for the understanding of collective phenomena in the interaction of light and matter.

In this Letter we report on the experimental realization of Bragg diffraction in an optical lattice, which for the first time lets us investigate the long range periodic order. We scatter blue radiation off rubidium atoms bound in a body-centered cubic lattice induced by a near infrared optical standing wave. The side of the conventional cubic cell is given by the wavelength λ_r of the trapping field, and the reciprocal lattice is spanned by the basis $\mathbf{b}_1 = k_r(\hat{\mathbf{x}} - \hat{\mathbf{z}})$, $\mathbf{b}_2 = k_r(\hat{\mathbf{y}} - \hat{\mathbf{z}})$, and $\mathbf{b}_3 = 2k_r\hat{\mathbf{z}}$, where $k_r = 2\pi/\lambda_r$ [9]. $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$ denote the Cartesian unit vectors. Bragg diffraction occurs when the difference $\Delta\mathbf{k}$ between the incident and the outgoing wave vectors equals a reciprocal lattice vector, i.e., $\Delta\mathbf{k} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$, where n_i are integers. If we restrict ourselves to an incident light beam (wavelength λ_b) propagating within the horizontal x - y plane (i.e., $2n_3 = n_1 + n_2$), the Bragg condition can be written $2\lambda_r \cos\theta = \lambda_b(n_1^2 + n_2^2)^{1/2}$, where θ denotes the angle between the incident wave vector and the normal of the lattice plane. If we adjust the incident wave vector according to the Bragg condition for the [201] planes of our optical lattice (in standard notation [10]), we observe reflection of the incident light into a diffraction limited Bragg beam. Since the atoms vibrate around their equilibrium positions, the background of incoherent scattering is raised and the Bragg diffracted intensity is decreased as described by the Debye-Waller factor [10]. Nevertheless, the intensity of the Bragg beam exceeds the incoherently scattered background by orders of magnitude.

Previous experiments have investigated the elastic scattering from optical lattices with light beams which had the same frequency as the trapping field [11,12]. These experiments were mainly sensitive to a four-wave mixing process which probes the polarizability in the atomic medium induced by the interference between the incident

probe beam and the trapping field. From such experiments no direct information could be obtained about the long range periodic order of the atomic lattice itself. In our experiment, the scattered light beam has a frequency which is nearly a factor of 2 higher than that of the trapping field. The rapidly oscillating interference pattern between the probe and the lattice field therefore has no influence on the atomic motion. The scattering process is determined entirely by the structure of the optical lattice.

We can describe Bragg diffraction by a simple model assuming each atom being bound to a harmonic potential centered at some lattice site $\mathbf{R}$ with a root mean square extension of the wave function δR . We consider a linearly polarized plane traveling wave with intensity I to be incident on the atomic sample. The power dP diffracted into the solid angle $d\sigma$ is then given by the far-field expression

$$\frac{dP}{d\sigma} = \left(\frac{k_b^2}{4\pi} \right)^2 I \sin^2(\xi) |\alpha|^2 \exp(-2W) \left| \sum_{\mathbf{R}} e^{i\Delta\mathbf{k} \cdot \mathbf{R}} \right|^2, \quad (1)$$

where ξ is the angle between the diffracted wave vector and the polarization vector of the incident beam, and α denotes the atomic polarizability at the incident wavelength. The Debye-Waller factor $W = \frac{1}{6}(\Delta\mathbf{k})^2(\delta R)^2$ accounts for the mean spatial atomic extension in the potential well [10]. The sum in the structure factor on the right of Eq. (1) has to be taken over all lattice vectors $\mathbf{R}$ which are populated by an atom. When $\Delta\mathbf{k}$ satisfies the Bragg condition, the structure factor becomes equal to the square of the number of irradiated atoms N . If N is sufficiently large, the angular width $\delta\theta$ of the Bragg resonance is given by the number of irradiated lattice sites independent of the degree of occupancy. The angular breadth is thus diffraction limited by the diameter d of the irradiated atomic sample, i.e., $\delta\theta \sim \lambda_r/2d$ [4].

As described in detail in Ref. [13], we prepare a three-dimensional spin-polarized lattice of the rubidium isotope ^{85}Rb in the intersection of three mutually orthogonal standing light waves ($\lambda_r = 780.2$ nm) which define the $\hat{x}$, $\hat{y}$, and $\hat{z}$ directions, respectively. We adjust the polarizations of the lattice beams and the time phase differences such that the atoms are arranged in a cubic body-centered geometry with orientation of their spins along the vertical z axis. The detuning of the lattice field from the atomic transition $5S_{1/2}(F=3) \rightarrow 5P_{3/2}(F'=4)$ (F is the total angular momentum) is typically -10Γ (Γ is the decay rate of the excited state) and the antinode Rabi frequency is 7Γ , which yields a potential depth of several MHz. In the harmonic approximation, the oscillation frequency of deeply bound atoms is $\Omega \approx 180$ kHz. The trapped atoms are optically pumped into the outermost ground state sublevel ($F=3, m_F=+3$). The experiment proceeds in two alternating steps. We first load a cold and dense sample of 10^7 atoms from the background vapor into a magneto-optical trap (MOT) producing an atomic cloud of ≈ 1.5 mm in diameter.

After 250 ms the MOT is switched off for 30 ms and the atoms are arranged in the optical potentials created by the six lattice beams (diameter 5 mm) which are also present during the MOT phase.

For Bragg diffraction we use a blue light beam tuned near to the $5S_{1/2}(F=3) \rightarrow 6P_{1/2}(F'=2 \text{ or } F'=3)$ transition at $\lambda_b = 421.7$ nm in order to enhance the scattering cross section. We generate the tunable monochromatic blue light (bandwidth < 1 MHz) by frequency doubling of a grating-stabilized diode laser. The experimental setup is sketched in Fig. 1. We use only $30 \mu\text{W}$ in a collimated beam of 3 mm diameter (divergence 0.24 mrad) in order to avoid large radiation pressure on the trapped atoms which would cause a loss of atoms. We choose the [201] lattice planes (normal to $\hat{x}$), for which the Bragg condition is satisfied at $\theta = 57.3^\circ$. In order to vary this angle over several degrees without affecting the overlap with the optical lattice, the coupling mirror M is imaged onto the optical lattice (cf. Fig. 1).

When the Bragg condition is matched we observe a strong increase of the scattered intensity by at least 3 orders of magnitude as compared to the background of diffuse scattering. The signal disappears when the time phase differences are set to values for which no optical lattice is formed, or when the MOT field is superposed on the optical lattice. In neither of these cases do we observe discrete vibrational levels of the atomic motion, which indicates that the increase of the scattered light is related to strong atomic confinement in the potential wells. In Fig. 2 we show spectra of the diffracted intensity at 421.7 nm. If the incoming light is linearly polarized in the horizontal plane [σ polarization, Fig. 2(a)], two resonances appear at the frequencies of the two hyperfine transitions from the ($F=3$) ground state to the ($F'=2$) and ($F'=3$) excited state levels, respectively. The different size of the resonances reflects the line strength ratio of 1:5. When the polarization is rotated by 90°

FIG. 1. Scheme of the Bragg diffraction experiment. The pattern of dots represents the sparsely populated atomic lattice. The diffracted light is detected at a distance of 21 cm by a photomultiplier (PM) with variable aperture. A photodiode (PD) monitors the transmission of a probe beam at 780 nm.

FIG. 2. Spectrum of the Bragg diffracted intensity versus frequency of the incident blue light. The incident beam is linearly polarized (a) in the horizontal plane (σ polarization) and (b) along the vertical direction (π polarization). The resonance frequencies of the $5S_{1/2}(F=3) \rightarrow 6P_{1/2}(F'=2)$ and ($F'=3$) transitions are indicated above.

[π polarization, Fig. 2(b)], the disappearance of the resonance at lower frequency shows that only spin-polarized atoms contribute to the Bragg diffraction signal, since only the Zeeman component ($F=3, |m_F|=3$) of the ground state does not couple to the excited state ($F'=2$) for π -polarized light.

We determine the dependence of the total diffracted power on the incidence angle by tilting the coupling mirror M and detecting the total diffracted power with an aperture of 8 mm diameter in front of the photomultiplier. We observe a resonance with a full width at half maximum of 0.26 ± 0.02 mrad, which is still limited by the collimation of the incident beam. By taking into account the actual experimental geometry we infer from the measured angular breadth that the diameter of the optical lattice has to be larger than 1.5 mm. The extension of the lattice thus exceeds the initial atomic distribution in the MOT, suggesting an atomic drift motion inside the lattice [12] such that the atoms tend to populate a large fraction of the available lattice sites. Further improvement of the resolution will allow us to study the drift in more detail.

We now estimate the total power P diffracted into the Bragg beam in the case of π polarization [i.e., $\sin(\xi) = 1$]. The blue intensity incident on the optical lattice is $800 \mu\text{W}/\text{cm}^2$. We assume a total number N of approximately 10^7 atoms which we have determined by fluorescence measurements, and a temperature of $15 \mu\text{K}$ [corresponding to a localization $\delta R/\lambda_r = 0.08$ and $\exp(-2W) = 0.76$ in the harmonic approximation for the potential], which we have extracted from probe transmission spectra. Integration of Eq. (1) yields $P \approx 1 \mu\text{W}$ to be diffracted at resonance into the Bragg spot. We actually measure $P = 60 \text{ pW}$ with an uncertainty of 50%, which differs by 1 order of magnitude from the value predicted by Eq. (1). The main cause for this discrepancy we attribute to the assumption of a thermal

equilibrium distribution for the estimation of δR which is not necessarily fulfilled in optical lattices, since the atoms permanently interact with the lattice field. Improved models are needed to derive the mean spatial extension of the atomic wave packet. The exponential dependence of P on the square of both δR and $|\Delta \mathbf{k}|$ can be exploited for a direct measurement of the degree of atomic localization by comparing the power diffracted into two different Bragg spots. This technique will also circumvent the problem of accurately determining the number of bound atoms N and the polarization α in Eq. (1), since these terms cancel when two spots are compared.

To study the motion of atoms deeply bound in the potential wells we combine Bragg diffraction with an additional weak probe beam at 780 nm. When the frequency difference between the probe and the lattice field matches the energy separation between vibrational states (divided by Planck's constant), photons are exchanged between the lattice and the probe field due to induced Raman transitions between different vibrational states [14]. These transitions lead to amplifying (absorbing) resonances in the probe transmission when the probe frequency is below (above) the lattice field frequency [see spectrum in Fig. 3(b)]. In both cases population is transferred from lower to higher lying vibrational levels, which is equivalent to an increase of δR . From the sensitive dependence of the Debye-Waller factor on δR one expects a strong decrease of the Bragg diffracted intensity when a Raman transition is induced by the infrared probe. In particular, when the probe beam is sufficiently weak, i.e., the transition rate is small, it will only modify the equilibrium population of the lowest vibrational states which (due to the Lamb-Dicke effect) display small relaxation rates [14], while the probe induced population transfer involving higher lying states is practically inhibited by their strong relaxation. Bragg diffraction in the presence of an additional probe therefore allows one to selectively address only the lowest lying vibrational levels. This contrasts the case of the probe transmission spectrum to which generally a large number of vibrational levels contribute [13,14].

We show this effect in Fig. 3, where we compare the Bragg diffracted intensity [Fig. 3(a)] with the transmitted probe intensity [Fig. 3(b)] as the probe frequency is scanned. We clearly see that the resonances in the diffracted signal are much narrower (particularly at $\pm 2 \Omega$) and exhibit no anharmonicity (i.e., the second resonance appears exactly at $\pm 2 \Omega$) in contrast to the probe transmission spectrum. The probe intensity was adjusted to yield a Rabi frequency for the coupling of adjacent vibrational levels (at $\pm \Omega$), which is on the order of the relaxation rate of the vibrational ground state ($\approx 30 \text{ kHz}$). The Rabi frequency of Raman transitions exchanging two vibrational quanta (at $\pm 2 \Omega$) is 1 order of magnitude smaller. Thus, mainly the ground state contributes to the Bragg spectrum, especially for the resonances at $\pm 2 \Omega$. The resonant decrease of the scattered intensity by as

FIG. 3. (a) Infrared probe induced resonances of the Bragg diffracted intensity at fixed blue frequency. The intensity is given in relative units (1 denotes the diffracted intensity without probe). The abscissa shows the frequency difference between the probe and the lattice field in units of the vibrational frequency Ω . (b) Corresponding transmission spectrum of the probe beam.

much as 20% demonstrates the dominant contribution of deeply bound atoms to Bragg diffraction [Fig. 3(a)]. In contrast, the important contribution of higher lying (and thus spectrally broader and more closely spaced) vibrational levels to the probe transmission spectrum becomes apparent by the broadening observed in the Raman resonances and by the fact that the resonance frequency of the second sideband is smaller than 2Ω [14] [Fig. 3(b)]. The different sensitivity of the Bragg spectrum and the probe transmission spectrum on the deeply bound atoms also becomes visible when we heat the lattice by tuning the lattice field frequency closer to resonance. In this case the Bragg signal completely vanishes, while the transmission spectrum is still preserved showing significantly broadened Raman resonances.

In summary, we have demonstrated Bragg diffraction from an optical lattice, thus for the first time directly revealing the long range spatial order. From the angular breadth of the Bragg diffraction we deduce a lower bound for the size of the optical lattice, i.e., the range over which the periodic order is preserved. We also have shown how Bragg diffraction can be used as a tool to selectively study the motion of atoms deeply bound in the potential wells. The comparison of Bragg diffraction for different Bragg angles should allow one to accurately determine the localization of the atoms and to analyze possible deviations from a random atomic distribution. This technique should be applicable also in the limit of far detuning, which is a promising regime for optical lattices not yet experimentally explored. Bragg diffraction offers a novel way to investigate the trapping mechanism

in optical lattices by studying the second-order time correlation of the diffracted signal which reflects typical time scales during which the atoms are bound at a particular lattice site before drifting or tunneling to another potential well. Another intriguing application for Bragg diffraction is the exploration of optical lattices to study multiple light scattering effects, since the periodic arrangement of atoms in the near resonant light field represents a unique model system [6,15].

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