The pump–probe coupling of matter wave packets to remote lattice states

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Abstract. The coherent manipulation of wave packets is an important tool in many areas of physics. We demonstrate the experimental realization of quasi-free wave packets of ultra-cold atoms bound by an external harmonic trap. The wave packets are produced by modulating the intensity of an optical lattice containing a Bose–Einstein condensate. The evolution of these wave packets is monitored in situ and their six-photon reflection at a band gap is observed. In direct analogy with pump–probe spectroscopy, a probe pulse allows for the resonant de-excitation of the wave packet into states localized around selected lattice sites at a long, controllable distance of more than 100 lattice sites from the main component. This precise control mechanism for ultra-cold atoms thus enables controlled quantum state preparation and splitting for quantum dynamics, metrology and simulation.

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1. Introduction

Wave packets—non-stationary superpositions of energy states—have held a special place in physics ever since Schrödinger showed that a superposition of states can form a spatially localized entity evolving in a manner similarly to a classical particle [1]. Despite being ubiquitous in nature, wave packets remained an elusive concept for decades. The advent of ultra-short laser pulses has, however, enabled a multitude of observations of wave packet phenomena, e.g. in highly excited atomic Rydberg states [2, 3], molecular states [4–8] and semiconductor systems [9].

One of the main applications of wave packets in these systems has been the investigation of complex quantum systems using the so-called pump–probe spectroscopy [4, 6, 8, 9]. An initial short pump pulse creates an excited state wave packet, which is allowed to evolve for a variable duration. Subsequently, a probe pulse interrogates this dynamic evolution by transferring it to a chosen final state. This process can thus provide information about coherent dynamics in the excited state [7, 10]. It can also be used for interferometry [11] or for the preparation of a desired final state [12], but to date it has not been employed for the investigation of ultra-cold atoms.

Meanwhile, the precise control of matter waves in Bose–Einstein condensates (BECs) has enabled a new field of wave packet manipulation [13]. Most experimental realizations in this field can be roughly divided into two categories. In the first type of experiments, wave packets propagating in free space [14], in a harmonic trap [15] or in wave guides [16] are exposed to brief pulses of optical lattice light, resulting in a controlled splitting of the cloud. In the second type, the atoms interact with the lattice light sufficiently long for tunnelling—conventionally under the constant force of gravity—to induce wave packet motion [17–19].

In contrast to previous realizations, we create quasi-free wave packets with energy above the lattice threshold and observe their motion in the combination of the lattice and a weakly confining potential in-situ. The oscillatory motion shows only limited spreading, indicating phase coherence in the individual eigenstates forming the wave packet [20]. The structural complexity arising from the combination of several bound and continuum states furthermore allows us to extend the highly successful pump–probe methodology to the regime of ultra-cold atoms by creating, monitoring and de-exciting matter wave packets in an optical lattice.

Using this pump–probe approach, we realize the first dynamic transfer into localized lattice states [21, 22] separated from the original cloud by more than 100 lattice sites. This mechanism
Figure 1. (a) Spectrum of the one-dimensional (1D) single-particle Schrödinger equation for the combined harmonic ($\omega_{\text{trap}} = 2\pi \times 37.9$ Hz) and periodic potential at a lattice depth $s = 16$. Each horizontal line represents the summed population density of the eigenstates within the respective energy bin. The darkness of blue increases with density and white indicates forbidden regions. The dashed red line indicates the local maximum of the lattice potential. Using a short pulse of lattice amplitude modulation, quasi-continuum wave packets are created (1), and subsequently oscillate in the potential (2). An appropriately timed second modulation pulse can de-excite the wave packets into localized states (3). (b) The same process is represented in the first Brillouin zone. (c) Sketch of the experimental setup. A magnetic trap provides a harmonic confinement and an amplitude modulated vertical lattice enables the wave packet dynamics. The lattice is not drawn to scale.

also allows for the transfer of controllable fractions of the cloud into several distinct localized states by using multiple probe pulses. Thus, it enables controlled quantum state preparation and splitting, with perspectives for quantum dynamics, metrology and simulation.

2. The single-particle Schrödinger spectrum

The wave packets are created in a combination of a 1D optical lattice along the vertical direction and a weak harmonic confinement

$$V(y) = \frac{1}{2}m\omega_{\text{trap}}^2y^2 - V_{\text{Lat}}\cos^2(k_Ry)(1 + \epsilon \cos(2\pi v_{\text{mod}}t)),$$

where $m$ is the mass of the atoms, $V_{\text{Lat}}$ is the lattice depth, $k_R = 2\pi/\lambda_{\text{Lat}}$ and $\lambda_{\text{Lat}}$ is the wavelength of the lattice light. In addition, we allow for a periodic modulation of the lattice depth with relative amplitude $\epsilon$.

The creation of wave packets can be visualized using the energy spectrum of the single-particle Schrödinger equation in the combined harmonic and optical lattice potential [21, 22]. This spectrum is shown in figure 1(a), where the discrete eigenfunctions have been squared.
and summed subsequently within equidistant energy bins. In this representation, darker shades of blue represent higher density. At a given spatial location it reflects the conventional band structure characterized by discrete bands separated by energy gaps. To a good approximation, the spectrum therefore consists simply of pseudo-bands shifted according to spatial dependence of the confining harmonic potential. This spectrum allows for a good understanding of the dynamics described below.

In our realization the depth of the 1D optical lattice \( V_{\text{Lat}} \) is chosen such that states up to the second excited band are bound in the lattice and isolated by band gaps. The states in bound bands outside the trap centre are confined to narrow regions in space, resulting in the so-called localized states. Tunnelling between these states is inhibited due to the harmonic site-to-site energy shift. In contrast, eigenstates above the lattice threshold form a quasi-continuum of states delocalized over a large distance. A harmonic modulation of the lattice depth with a frequency \( v_{\text{mod}} \) close to the transition frequency from the lowest band to the second excited band, \( v_{02} \), can induce transitions between these bands \([23]\). Further modulation drives the population into the quasi-continuum states that exist above the threshold of the lattice.

3. The experimental creation of quasi-free wave packets

Our experimental system \([24]\) consists of a BEC in a harmonic magnetic potential and a 1D optical lattice in the vertical direction (figure 1(c)). A BEC of \(^{87}\text{Rb}\) atoms in the \( 5^2S_{1/2}|F = 2, m_F = 2\rangle \) state is prepared in a quadrupole-Ioffe magnetic trap. After condensation, the magnetic potential is considerably relaxed to obtain trap frequencies of 12.3 and 37.9 Hz in the axial and radial directions, respectively. Pure condensates of approximately \( 1 \times 10^5 \) atoms are then loaded adiabatically into the vibrational ground state of a 1D optical lattice. The optical lattice is formed along the vertical axis (one of the radial directions of the trap) by a retro-reflected laser beam at a wavelength of \( \lambda_{\text{Lat}} = 914 \text{ nm} \) with a \( 1/e^2 \) waist of 120 \( \mu\text{m} \). For all experiments the lattice depth was \( s = V_{\text{Lat}}/E_R = 16 \), where \( E_R = h^2/(2m\lambda_{\text{Lat}}^2) \).

To produce the wave packets experimentally, the lattice amplitude is modulated \([25]\) in a short (500 \( \mu\text{s} \)), large-amplitude (\( \epsilon = 0.3 \)) pulse at a modulation frequency of \( v_{\text{mod}} = 31 \text{ kHz} \) close to the transition frequency from band 0 to band 2, \( v_{02} = 30.5 \text{ kHz} \). This duration is chosen to be slightly longer than the \( \sim 250 \mu\text{s} \) needed for saturating the transfer into the quasi-continuum states \([26]\). Subsequently, images of the resulting clouds are taken \textit{in situ} following a variable evolution time. Two wave packets, travelling in each lattice direction away from the original cloud, are observed as shown in figure 2(a). The wave packets each contain roughly 2\% of the total atoms and do not show significant spreading as they travel to the turning point, are reflected and return. This behaviour is in agreement with a single-particle simulation and reflects the phase coherence in the individual eigenstates forming the wave packet \([20]\) rather than an interaction-induced soliton effect. Figure 2(a) shows the distance of the wave packet from the centre of the main component as a function of the evolution time during the first half of the oscillation period. It reveals a time to reach the turning point of roughly \( t_{\text{turn}} = 2.6 \text{ ms} \) (\( t_{\text{turn}} = 3.0 \text{ ms} \)) for the upper (lower) peaks. We stress that this observation is inconsistent with harmonic oscillation at the trap frequency \( \omega_{\text{trap}} = 2\pi \times 37.9 \text{ Hz} \) from which we would expect a turning point at 6.6 ms. In the following paragraphs, we show that this effect is due to Bragg reflection. The influence of gravity does not modify the dynamics of the wave packet to first order, since the combination of gravity and the harmonic confinement merely shifts the location of the minimum of the combined potential. This is in strong contrast to the Wannier–Stark
Figure 2. Propagation of the wave packets after excitation with a 500 µs modulation pulse. (a) Position of the upper (×) and the lower (○) wave packet as a function of the evolution time after modulation. All experimental images were rotated 90° counter-clockwise for clarity. (b) Wave packet dynamics obtained from a numerical simulation (see text).

work performed using the lattice potential and gravity alone [17–19]. The influence of gravity does, however, introduce a small anharmonicity into the potential in our system, which modifies the motion of the wave packet travelling upwards slightly compared to the one travelling downwards. For the quantitative analysis, in the following we use the upper component only.

An intuitive understanding of the process can be obtained from an analysis based on figure 1(a) and the conventional band structure represented in the first Brillouin zone in figure 1(b). The modulation pulse transfers a small fraction of the ground state population via a two-step excitation to a superposition of quasi-continuum states, determined by the individual coupling matrix elements. In the band picture, this is equivalent to a transfer into the fourth excited band for the chosen lattice depth. Energy and momentum conservation dictates a transfer into states with opposite quasi-momentum $\pm \hbar q_{\text{max}}$, where $4 \leq q_{\text{max}} / k_R \leq 5$ and $k_R = 2\pi / \lambda_{\text{Lat}}$. The wave packets subsequently exchange their initial kinetic energy for potential energy by moving outward in the harmonic potential while rolling down the appropriate bands. When the first significant band gap is encountered, their direction is reversed due to a high-order Bragg reflection [27].

This interpretation directly allows for a simple calculation of the expected behaviour of the wave packets. Treating the quasi-momentum $\hbar q$ as the momentum $p$ of a classical particle moving in a harmonic trap

$$p(t) = \hbar q_{\text{max}} \cos(\omega_{\text{trap}} t),$$

(2)
the times at which the quasi-momentum passes the avoided crossings between bands $n$ and $(n-1)$ at $q = nk$, are

$$t_n = \arccos \left( \frac{nk}{q_{\text{max}}} \right) / \omega_{\text{trap}}$$

for $0 \leq n < 4$. Quantitatively, we obtain $t_3 = 3.0$ ms for $q_{\text{max}} \sim 4k_R$ in good agreement with the experimental result and therefore interpret the reflection of the wave packet as a Bragg reflection on the gap between the second and the third band (six-photon Raman process). A calculation of the Landau–Zener tunnelling probability confirms this, since it is essentially zero at $s = 16$ [27]. We have verified this interpretation by increasing the modulation frequency and observing that the wave packets propagate further due to the larger initial momentum.

For a more detailed understanding, we have also performed a single-particle numerical simulation of the process by solving the time-dependent Schrödinger equation in the combined potential. After the modulation pulse we obtain the wave packet as a superposition of eigenstates. The ensuing wave packet dynamics, dictated by the relative phase evolution of these states, is shown in figure 2(b) and reveals a turning point at 3.2 ms. We stress that the simulation neglects interactions and starts in the absolute single-particle ground state. In order to obtain qualitative agreement with experiment the simulation has to be performed at a significantly lower modulation frequency (28 kHz) compared to the experimental case. We attribute this mainly to the interaction-induced broadening of the initial state. In both cases the modulation amplitude was $\epsilon = 0.3$.

**4. The pump–probe creation of localized states**

The production process of wave packets described above bears a strong resemblance to the pump pulse in a pump–probe experiment. We therefore illustrate the dynamical control of these wave packets by coupling them into outlying localized states [21, 22] with a second (probe) modulation pulse. This realizes the first dynamic population and *in-situ* detection of such states. Unlike related experiments [19, 22, 28], our method allows for the transfer of a controllable fraction of the wave packets into states that are separated by large distances ($\sim 100$ sites) from the original cloud. It is thus related to the topic of controlled transport in tilted optical lattices, which has recently been investigated theoretically [29, 30].

The condition for the population of the outlying localized states can be understood by returning to figure 1. After some evolution time the wave packets have a spatial overlap with localized states at an energy difference of $h\nu_{\text{mod}}$. A brief modulation pulse will then induce coupling to these states in correspondence to the Franck–Condon principle for transitions between vibrational states. Appropriate probe frequencies indeed allow for de-excitation into distinct localized states in each low-lying band. We have verified this by varying the probe frequency at a fixed wave packet evolution time [26]. For simplicity, however, we primarily show results using the same frequency for the pump and the probe pulses.

Experimentally, we investigate the transfer using a 500 $\mu$s probe pulse after variable evolution times. As shown in figure 1 energy conservation dictates which bands are accessible, and at the given modulation frequency only the first band can be populated. The resulting population for the upper peak is shown in figure 3(a). We observe a double peaked resonance structure corresponding to the first passage and subsequent return of the wave packet following the reflection (around $t = 3$ ms). In addition, we observe a second double peaked resonance after
Figure 3. Time dependence of the pump–probe spectroscopy. (a) Measured population in the localized states (first excited band) as a function of the delay between the 500 µs pump and probe pulses ($\nu_{\text{mod}} = 32$ kHz) (solid dots). The double peaked structure around $t = 3$ ms corresponds to the passage of the wave packet through the resonance region. Representative error bars are included at $t = 1.75$ ms and at $t = 6.75$ ms. (b) Numerical simulation of the pump–probe experiment (see text) (open circles). In both cases the solid line is a cubic spline as a guide to the eye.

approximately 10 ms, corresponding to the wave packet that has completed $3/4$ of an oscillation after originally travelling downwards. We have realized up to 80% de-excitation efficiency, and by varying the duration of the probe pulse the transfer can be adjusted freely, allowing, for instance, for a 50/50 splitting. The localized states are observed to be stationary for more than 200 ms and the band gap is sufficiently large to ensure that they remain within the first band.

To model the pump–probe dynamics theoretically, we extend the numerical simulation discussed above by adding a second modulation pulse after a variable delay. For each delay, we obtain the distribution among all eigenstates. To extract the bound state population we identify the eigenstates with energies roughly $h\nu_{\text{mod}}$ above the ground state and plot only the contribution from the outlying positions. The result of this numerical model is shown in figure 3(b). Although interaction effects are neglected, the numerical results show qualitatively the same features as the experimental data, i.e. the double peak corresponding to the passage of the first wave packet and the double peak associated with the second wave packet having travelled $3/4$ of a full oscillation. We attribute the quantitative disagreement in the location of the structures mainly to the fact that the numerical simulations are performed at a slightly different frequency (28 kHz) as discussed above. In addition, the large difference in the vertical scales of the experimental and theoretical data shows that the efficiency of the process cannot be explained quantitatively within the single-particle model.
Figure 4. Positions of the populated localized states as a function of lattice modulation frequency. Dots (circles) represent localized clouds in the first (second) excited band. The fits correspond to the expected square root behaviour (see equation (4)).

5. Steady state population of localized states

Finally, the position of the localized states was systematically investigated for various modulation frequencies around the transition frequency $\nu_0$ (see figure 4). In this case 10 ms modulation pulses were used to reach a steady state population in the localized states. The position clearly moves outwards as the frequency is increased and on the high-frequency side of the resonance a new set of close-lying components appears. The inset of figure 4 shows an image recorded at a modulation frequency of 36 kHz, displaying the main cloud and the inner and outer sets of localized states.

From figure 1(a) it is clear that at modulation frequencies $\nu_{\text{mod}} \geq \nu_0$ population can be coupled both to the first and the second excited bands, thus resulting in the two observed sets of populated outlying states. The position of each of these states, $x_i$, can be obtained by considering the energy balance between the modulation, the band and the harmonic potential energies

$$2h\nu_{\text{mod}} = h\nu_{\text{mod}} + h\nu_0 + \frac{1}{2}m\omega_{\text{trap}}^2 x_i^2,$$

where $\nu_0 = 0$. From this we obtain the expression for the localized state position $x_i = \sqrt{2h(\nu_{\text{mod}} - \nu_0)/m\omega_{\text{trap}}^2}$. Fitting the data of figure 4 to this functional dependence allows us to attribute the upper and the lower branch to the first and second bands, respectively. From the fit we obtain $\nu_{01}^{\text{fit}} = 18.5(2)$ kHz and $\nu_{02}^{\text{fit}} = 33.06(17)$ kHz, in good agreement with the first (18.1–19.3 kHz) and second (30.6–37.2 kHz) Bloch bands at $s = 16$. This agreement confirms that the process is well understood and demonstrates its applicability for the production of localized clouds in the lattice at a long distance from the central component.
Figure 5. Individual addressing of localized states. (a) Population of localized states after a modulation for 10 ms at 30 kHz. RF removal of (b) the main and (c) the main and lower components. (d) Population of multiple localized states with two probe pulses.

6. Outlook and conclusion

The efficient population of localized lattice states offers avenues for, for example, interferometric experiments. These require the ability to manipulate the localized states independently. To demonstrate this ability, we have implemented the radio-frequency (RF) removal of selected atoms similarly to [22]. Due to the gravitational potential, the condensate is shifted slightly downwards compared to the magnetic field zero. This gravitational sag in the weak magnetic confinement $x_{sag} = g/\omega_{trap}^2 = 173 \, \mu m$ is large enough to ensure that each cloud is located in a unique magnetic field. Selected peaks can thus be removed by applying an appropriate RF field to couple them to unbound magnetic states (see figure 5). This represents an ideal starting point for future investigations of the coherence properties of the localized states. It also enables new experiments that probe nonlinear matter wave dynamics, including the reflection and transmission of a wave packet on a BEC [31], the collision of wave packets and the investigation of their dispersive properties.

A particularly promising experimental extension is the use of multiple modulation frequencies. On the one hand, this will allow for a full analysis of the Franck–Condon-type overlap between bound and quasi-continuous states. On the other hand, it will enable the controlled population of many, spatially separated lattice states. We have indeed realized the general splitting of a single propagating wave packet into multiple distinct localized states by sequentially applying probe pulses at different frequencies (see figure 5 and [26] for more details). Furthermore, we have observed the coupling of the wave packet into higher excited states [26]. This allows for a rich dynamics, and it will be interesting to study, for example, the coherence of each individual step and to what extent coherent control techniques [20] can be utilized to realize near-unity efficiencies.

If the pump–probe mechanism can be combined with single site addressing [32], it may be possible to controllably place two atoms in the same well but in separate bands, forming...
the basis of a two-qubit gate. As a first step in this direction we have created localized clouds containing an equal mixture of the first and second excited bands by choosing an appropriate modulation amplitude. The preparation of localized states in well-defined bands may also serve as a particularly pure source of atoms in selected bands. This topic has received considerable attention, since it will enable the investigation of the rich structure of extended Bose–Hubbard Hamiltonians including, for example, the supersolid state [33]. Recent theoretical proposals [34–36] predict transfer efficiencies of 95–99.9%; however, experimental preparation has been limited to 90% [35, 37]. In contrast, our preparation scheme produces extremely pure samples in selected bands since the localized states in our approach are spatially separated from the original cloud.

In conclusion, the experimental realization of quasi-free wave packets of ultra-cold atoms based on excitations in a combined optical lattice and harmonic trap has been demonstrated. Furthermore, a probe pulse in direct analogy with pump–probe spectroscopy allowed for the resonant de-excitation of the wave packets into localized lattice states at a controllable distance of more than 100 lattice sites from the main component. Finally, independent manipulation of the population of the localized states was implemented. The precise control of the external degrees of freedom thus makes these wave packets a versatile tool both for fundamental investigations and for applications in the field of lattice gases.

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