Strongly interacting atoms and molecules in a 3D optical lattice

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Abstract
We report on the realization of a strongly interacting quantum degenerate gas of fermionic atoms in a three-dimensional optical lattice. We prepare a band-insulating state for a two-component Fermi gas with one atom per spin state per lattice site. Using a Feshbach resonance, we induce strong interactions between the atoms. When sweeping the magnetic field from the repulsive side towards the attractive side of the Feshbach resonance we induce a coupling between Bloch bands leading to a transfer of atoms from the lowest band into higher bands. Sweeping the magnetic field across the Feshbach resonance from the attractive towards the repulsive side leads to two-particle bound states and ultimately to the formation of molecules. From the fraction of formed molecules we determine the temperature of the atoms in the lattice.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Quantum degenerate atomic gases in optical lattices offer the possibility of studying quantum many-body physics with unprecedented purity. Interacting atoms in optical lattices are ideally suited to experimentally simulate the Hubbard model [1, 2]. For fermions this model is elementary to describe the quantum physics of electrons in a solid. It takes into account a single band of a static lattice potential and assumes the interactions to be purely local [3]. The fundamental parameters include the tunnel coupling between adjacent lattice sites, the atom–atom interactions and the dimensionality of the system. The fermionic Hubbard Hamiltonian reads

\[ H = -t \sum_{\langle j,k \rangle,\sigma} c_{j,\sigma}^\dagger c_{k,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow}, \] (1)

where \( t \) is the hopping matrix element and \( c_{j,\sigma}^\dagger \) and \( c_{j,\sigma} \) are the creation and annihilation operators for a particle in the spin state \( \sigma \) at lattice site \( j \), respectively. \( n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma} \) is
the number operator at lattice site $j$, and $U$ quantifies the strength of the on-site interaction between atoms in different spin states.

Despite its conceptual simplicity the Hubbard Hamiltonian has not been solved except in the one-dimensional situation and in very few special cases in higher dimensions. Therefore, experimentally simulating the Hubbard model with ultracold atomic gases in optical lattices is a fascinating possibility of exploring the phase diagram of this model. Both the tunnelling matrix element $t$ and the on-site interaction $U$ can be adjusted experimentally. Whereas the tunnelling mainly depends on the depth of the periodic potential, the on-site interaction is determined by the $s$-wave scattering length $a$ for a collision between two distinguishable fermions. The $s$-wave scattering can be modified by means of a magnetically induced Feshbach resonance [4] which allows us to access any value of the scattering length.

As a first step along the path of such an experimental simulation we study the Hubbard model in the low-tunnelling regime, where $t$ is small and particles are assumed to stay on their initial lattice sites for the duration of the experiment. In this configuration approximative solutions of this model are feasible [5–8]. In the Hubbard model the interactions between particles are parametrized only by the parameter $U$ regardless of the physical details of the interaction. In reality, however, the interatomic van-der-Waals interactions are much more complex and the relevance of these details for the Hubbard model must be investigated before unknown many-body quantum phases can be addressed. Moreover, the possibility of converting fermionic atoms into bosonic molecules offers new insights beyond what has been studied in condensed matter physics so far. The physics of two interacting particles in a tight harmonic trap is governed by several length scales. These are the characteristic length of the van-der-Waals interaction potential between the atoms, the effective range, the scattering length and the extension of the ground state in the oscillator potential.

2. Tuning interactions between atoms

In an atomic gas, interactions are mediated by scattering processes. Because of the Pauli principle, elastic $s$-wave scattering in a degenerate fermionic gas takes place only in spin mixtures or mixtures with other atomic species. Feshbach resonances, a phenomenon originally discussed in the context of nuclear physics [9], allow a tuning of the scattering properties in a binary collision between two atoms to arbitrary repulsive or attractive values [10]. This enables the creation of strongly interacting atomic quantum gases.

2.1. A simple model: two interacting atoms in a harmonic oscillator potential

The collision properties between atoms are modified if the atoms are subject to strong confinement. If the particles are confined to a length scale comparable to the scattering length between them, the known picture of two-particle bound states has to be reconsidered. Such a tight confinement can for example be realized in a three-dimensional optical lattice, where atoms are localized to the lattice sites and the interactions can be tuned by a Feshbach resonance.

For simplicity we approximate a single potential well of the lattice by a three-dimensional harmonic oscillator potential. This fundamental quantum mechanical model system has been studied theoretically and the eigenenergies have been calculated in various approximations [11–14]. The interaction between two particles in a harmonic oscillator affects only the relative motion between the particles. After separating off the mass-of-mass degree of freedom we
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Figure 1. Energy spectrum of two interacting particles in a three-dimensional harmonic oscillator potential which is given by equation (4) in the mass-of-mass frame [11]. The asymptotic energies at $a \to \pm \infty$ are indicated by the dashed lines.

find the Hamiltonian for the relative motion

$$H_{\text{rel}} = -\hbar^2 \nabla^2 + \frac{1}{2} \mu \omega^2 r^2 + V(r)$$

with the reduced mass $\mu = m/2$, the atomic mass $m$, the trapping frequency $\omega$, and the two-particle interaction potential $V(r)$. We assume s-wave interactions with a scattering length $a$, which can be modelled by a regularized pseudopotential interaction

$$V(r) = \frac{4 \pi \hbar^2 a}{m} \delta^{(3)}(r) \frac{\partial}{\partial r} r.$$  \hfill (3)

This problem can be solved analytically [11] and the eigenenergies are given by the implicit equation

$$\frac{a_{ho}}{a} = \frac{\sqrt{2}}{\Gamma(-E/2 \hbar \omega + 3/4)} \frac{\Gamma(-E/2 \hbar \omega + 1/4)}{\Gamma(1)},$$

where $a_{ho} = \sqrt{\hbar/m \omega}$ and $\Gamma(x)$ denotes the Gamma function. In figure 1 we show the eigenenergies as a function of the scattering length. For $|a|/a_{ho} \ll 1$ the deviation of the eigenenergy from the noninteracting system is linear in $a$, as one would have expected naively. However, for large scattering length the energy shift saturates at $\pm \hbar \omega$ with respect to the noninteracting case.

In reality, the atoms are interacting via a van-der-Waals potential which is not at all $\delta$-function like, but has a tail which drops off as $1/r^6$ for large distances. Naturally the question arises, whether the pseudopotential approximation is valid for the case of two atoms. The validity of the pseudopotential approximation depends on the various length scales involved in the problem. Generally speaking, a pseudopotential treatment is valid, as long as the characteristic range of the van-der-Waals interaction $\beta_6 = (2\mu C_6/\hbar^2)^{1/4}$ is small compared with $a_{ho}$ [12, 13]. This assures that the interatomic potentials are not modified by the confinement and the microscopic (i.e. atomic) physics is not altered. For our parameters with $\beta_6/a_{ho} < 0.1$ this is well fulfilled. In [12, 13] it is argued that one has to consider an energy-dependent pseudopotential, if the effective range $r_{\text{eff}}$ of the interaction becomes comparable to the scattering length $a$ or the ground state extension $a_{ho}$. Then the scattering length takes the form

$$a(E) = \left( \frac{1}{a} - \frac{1}{2 a_{ho} \hbar \omega a_{ho}} E r_{\text{eff}} \right)^{-1}.$$  \hfill (5)
The effective range can for the case of $^{40}$K be calculated to be \[ r_{\text{eff}} \approx \frac{\beta_6}{3} \left( -\frac{4\beta_6}{a} + \frac{8\pi \beta_6^2}{a^2\Gamma(\frac{3}{2})^2} + \frac{\Gamma(\frac{1}{2})^3}{\pi} \right) = 98a_0, \] (6)
which is the same order of magnitude as $\beta_6$ and $a_{bg}$.

3. Interacting fermions in a lattice

For strong interactions between the fermions a multi-band Hubbard model must be considered which takes into account a coupling between Bloch bands [7] and the conversion of pairs of fermionic atoms into bosonic molecules. The regime of Fermi–Bose conversion is not accessible in standard condensed matter systems and only recently the first steps to understand this mixed world of fermions and bosons have been undertaken theoretically [5, 6, 14]. However, multi-band Hubbard models are extremely difficult to solve [16] and often solutions can only be derived for the low-tunnelling limit. In this limit the lattice can be considered as an array of microscopic harmonic traps occupied with two interacting atoms in different spin states. In the limit of zero tunnelling the lowest Bloch band maps onto the lowest vibrational harmonic oscillator state and higher bands map to excited oscillator states. This allows us to apply the results from the previous paragraph to the optical lattice. Feshbach resonances [9] allow for a controlled manipulation of the atomic scattering properties by means of an external magnetic field. Sweeping a magnetic field dynamically changes the two-body potentials and the adiabatic creation and dissociation of molecules can be observed, depending on the direction the magnetic field sweep.

3.1. Interaction induced coupling between Bloch bands

We have investigated the behaviour of the atoms when sweeping across the Feshbach resonance from the low-field to the high-field side (see figure 2(a)) [17]. When using this direction of the sweep there is no adiabatic conversion to molecules, but a transfer of atoms into an excited vibrational level of the harmonic oscillator is expected. We start from a noninteracting gas deep in a band insulator regime with $V_x = 12E_r$ and $V_y = V_z = 18E_r$ and corresponding trapping frequencies of $\omega_x = 2\pi \times 50$ kHz and $\omega_y = \omega_z = 2\pi \times 62$ kHz in the individual potential minima. $E_r = h^2/(2m\lambda^2)$ denotes the recoil energy for a lattice laser with a wave length $\lambda$. We prepare a mixture of the two atomic states $|F = 9/2, m_F = -9/2\rangle$ and $|F = 9/2, m_F = -5/2\rangle$, which have a Feshbach resonance at a magnetic field of 224 G [18]. In the following we will refer to the atomic states only by the $m_F$ quantum number. Starting from the initial magnetic field of 210 G we ramp the magnetic field with an inverse sweep rate of 12 $\mu$s G$^{-1}$ to different final values around the Feshbach resonance. After turning off the optical lattice adiabatically and switching off the magnetic field we measure the momentum distribution which reflects the quasi-momentum distribution of the atoms in the lattice [17, 19]. The adiabatic switch-off process of the lattice adiabatically converts the quasi-momentum of the atoms in the lattice into momentum which can be observed in a time-of-flight image. To study the effect of the interactions we determine the fraction of atoms transferred into higher bands, which corresponds to excited states inside the individual lattice wells. For final magnetic field values well above the Feshbach resonance we observe a significant increase in the number of atoms in higher bands along the weak axis of the lattice, demonstrating an interaction-induced coupling between the lowest bands. The fraction of atoms transferred could be limited by the number of doubly occupied lattice sites and tunnelling within the higher bands. The fraction of doubly occupied lattice sites was determined in a different
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Figure 2. Interaction-induced transition between Bloch bands. (a) Illustration of the sweep across the Feshbach resonance. (b) Momentum distribution for a final magnetic field of \( B = 233 \) G and a 12 µs/G sweep rate. Arrows indicate the atoms in the higher bands. (c) Transferring fermions to higher bands using a sweep across the Feshbach resonance (filled symbols). The inverse magnetic field sweep rate is 12 µs/G. The line shows a sigmoidal fit to the data. The open symbols show a repetition of the experiment with the atoms prepared in the spin states \( |m_F = -9/2\rangle \) and \( |m_F = -7/2\rangle \) where the scattering length is not very sensitive to the magnetic field. The magnetic field is calibrated by rf spectroscopy between Zeeman levels. Due to the rapid ramp the field lags behind its asymptotic value and the horizontal error bars represent this deviation. Data are taken from [17].

experiment to be approximately 40% [20]. A recent theoretical work suggests that up to 75% of these atoms could be transferred into higher bands, which would result in a total fraction of 30% in higher bands [7], which is somewhat more than observed in our experiment.

3.2. Producing bosonic molecules from fermionic atoms

We now study the reverse sweep direction where pairs of atoms are transferred into deeply bound states [20]. This technique of adiabatic conversion of atoms into molecules [18] provides a useful way to generate ultracold molecular samples. The lowest branch of the energy spectrum in figure 1 is accessed by starting from a noninteracting Fermi gas but sweeping the magnetic field from the high-field towards the low-field side of the Feshbach resonance. This sweep adiabatically converts the atomic pairs into molecules. First we create a band insulator for each of the two fermionic spin states \( |-7/2\rangle \) and \( |-9/2\rangle \) in the optical lattice. Subsequently, the molecules are formed by ramping the magnetic field from the zero crossing of the scattering length at \( B = 210 \) G in 10 ms to its desired value close to the Feshbach resonance located at \( B_0 = 202.1 \) G [21]. We measure the binding energy \( E_B \) of the dimers by radio-frequency spectroscopy [18, 22, 23]. The idea of the rf-spectroscopy is shown schematically in figure 3(a): an rf pulse dissociates the molecules and transfers an atom from the state \( |-7/2\rangle \) into the initially unpopulated state \( |-5/2\rangle \) which does not exhibit a Feshbach resonance with the state \( |-9/2\rangle \) at this magnetic field. Therefore the fragments
Figure 3. Illustration of the rf spectroscopy between two bound states within the wells of the optical lattice. (a) The atoms in the initial states $|\pm 7/2\rangle$ (red) and $|\pm 9/2\rangle$ (black) are converted into a bound dimer by sweeping across a Feshbach resonance if lattice sites are doubly occupied. Application of an rf pulse on the transition $|\pm 7/2\rangle \rightarrow |\pm 5/2\rangle$. For singly occupied sites the rf resonance is at the bare atom transition given by the magnetic field. If a site is doubly occupied the rf transition dissociates the molecule. For this the binding energy $E_B$ has to be supplied and the rf resonance is shifted. (b) The rf spectrum taken at $B = 202.9\,\text{G}$, i.e. for $a < 0$, and a lattice depth of $22\,E_r$. The atom numbers are shown for the $|\pm 9/2\rangle$ (squares), $|\pm 7/2\rangle$ (circles) and $|\pm 5/2\rangle$ (triangles) states. The lines are Lorentzian fits to the data. Data are taken from [20].

after dissociation are essentially noninteracting and occupy the noninteracting ground state of the harmonic oscillator potential. We vary the detuning $\delta = \nu_{RF} - \nu_0$ of the rf pulse from the resonance frequency $\nu_0$ of the atomic $|\pm 7/2\rangle \rightarrow |\pm 5/2\rangle$ transition. The power and the duration of the pulse are optimized to constitute approximately a $\pi$-pulse on the free atom transition. The number of atoms in each spin state is detected using absorption imaging after ballistic expansion.

Figure 3(b) shows rf spectra of atoms and molecules trapped in a three-dimensional lattice with a potential depth of $V_0 = 22\,E_r$ corresponding to $\omega = 2\pi \times 65\,\text{kHz}$. The spectrum in figure 3(b) is taken at a magnetic field of $B = 202.9\,\text{G}$ where $a/a_{ho} = -1.3$. For negative scattering lengths, the molecules are only bound when they are strongly confined whereas no bound state would exist in the homogeneous case [24]. The spectrum exhibits two resonances: the one at $\delta = 0$ corresponds to the atomic transition from the $|\pm 7/2\rangle$ into the $|\pm 5/2\rangle$ state. This transition takes place at all lattice sites which initially were only singly occupied and no molecule can be formed. The second resonance at $\delta > 0$ corresponds to molecule dissociation and is shifted from the atomic resonance by the binding energy. Together with the increase in the $|\pm 5/2\rangle$ atom number we observe a loss of atoms in the $|\pm 7/2\rangle$ state, whereas the $|\pm 9/2\rangle$ remains unaffected. This is expected since the rampdown of the lattice before detection dissociates all molecules and the $|\pm 9/2\rangle$ atom number should be fully recovered.
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Figure 4. The measured binding energy of molecules in a three-dimensional optical lattice. The data are taken for several potential depths of the optical lattice of $6E_r$ (triangles), $10E_r$ (stars), $15E_r$ (circles) and $22E_r$ (squares). The solid line corresponds to the theory of [11] with no free parameters, the dashed line uses an energy-dependent pseudopotential according to [12]. At the position of the Feshbach resonance ($a \to \pm \infty$, horizontal dashed line) the binding energy takes the value $E = -\hbar \omega$. Data are taken from [20].

In contrast to earlier work on rf dissociation of molecules where the molecules were dissociated into a continuum and the fragments were essentially free particles [18, 22, 23] in our configuration the fragments occupy a discrete energy eigenstate of the confining potential. In such a bound–bound transition no extra kinetic energy is imparted onto the dissociated fragments and we determine the binding energy from the separation of the atomic and the molecular peak. Moreover, since there is at most one molecule present per lattice site, collisional shifts [25, 26] are absent and we can estimate the error in the binding energy from the fit error which is less than 5 kHz.

We have investigated the dependence of the binding energy of the molecules on the scattering length (figure 4). The scattering length is derived from the magnetic field using the parametrization of the Feshbach resonance $a(B) = a_{bg}(1 - \frac{\Delta B}{\Delta B_0})$, with $a_{bg} = 174a_0$ [27] and $\Delta B = 7.8$ G [28]. We compare our data with the theory for the binding energy of two particles trapped in a harmonic oscillator potential interacting via an energy-independent pseudopotential [11]. Depending on the scattering length the binding energy $E$ of the molecules varies according to equation (4). We have determined the ground state extension $a_{ho}$ by minimizing the energy of a Gaussian trial wave function inside a single well of our lattice potential. We find the normalized binding energy $E/\hbar \omega$ to be independent of the strength of the lattice and all data points to agree well with the theoretical prediction of equation (4) without adjustable parameters. However, a model with an energy-dependent pseudopotential [12] gives very similar results (dashed line in figure 4). Both models agree to within a few per cent, which is small compared to experimental uncertainties. Further improvements taking into account more details of the atom–atom interaction in a two-channel model have been suggested [13, 14] and could be tested with our data.

4. Thermometry in the optical lattice

In contrast to conventional condensed matter physics experiments atoms in optical lattices are subject to an inhomogeneous potential. This makes the concept of the ‘filling’ of the lattice
Figure 5. The measured molecular fraction as a function of the inverse scattering length at the end of the magnetic field sweep which is derived from the peak heights of the rf spectra and corrected by the overlap integral. We find a constant molecular fraction of $(43 \pm 5)\%$.

more subtle than in the homogeneous case. One possible way of quantifying the filling of the inhomogeneous lattice is to study the fraction of doubly occupied sites for a two-component Fermi gas. The fraction of doubly occupied lattice sites is closely related to the temperature of the atoms in the lattice and therefore it represents a useful way of determining the temperature of atoms in the lattice. This quantity is of importance for many proposed experiments in which phase transitions of fermions in lattices are studied, and special cooling techniques to reach these temperatures have been devised [2, 29–31].

In the tight binding regime molecules can only be formed, when two particles reside at the same lattice site. Therefore the measurement of the molecule formation gives access to the fraction of doubly occupied lattice sites. We assume that the magnetic field sweep across the Feshbach resonance is fast enough such that the atomic density does not change and we form molecules at all those lattice sites where two atoms reside. Using the rf dissociation technique we break up the molecules and determine the fraction of molecules from the spectra. The dissociation probability depends on the strength of the rf coupling, on the overlap between the initial and the final wave function and on the fraction of doubly occupied lattice sites. When we compare the spin-flip probability on the atomic transition and on the molecular transition, the rf coupling strength is equal, but the spatial overlap is different. For the atomic transition, the overlap is approximately unity since both, initial and final states correspond to the noninteracting ground state of the harmonic potential well. For the molecular peak we calculate the overlap integral

$$\left| \int d^3r \psi_{ho}(r)^* \psi_{l=0}(r) \right|^2$$

(7)

with $\psi_{ho} = \left( \pi a_{ho}^2 \right)^{-3/4} e^{r^2/2a_{ho}^2}$ being the oscillator ground state wave function. $\psi_{l=0}(r) = \frac{1}{2} \pi^{-3/2} A e^{-r^2/2a_{ho}^2} \Gamma(-\nu) U(-\nu, \frac{3}{2}, r^2)$ is the wave function of the bound state in relative coordinates [11] and $U(n, m, x)$ is the confluent hypergeometric function and $\nu = \frac{E}{2\hbar \omega} - 3/4$. We determine the relative height of the atomic and the molecular peak in the spectra (figure 3) and divide the value by the overlap integral. The resulting value gives the fraction of doubly occupied sites in the lattice (see figure 5).
In the tight binding limit we calculate the fraction of doubly occupied sites of the lattice for a given temperature. For the analytic calculation we start from the density of states given by

$$\rho_{3D}(E) = \frac{2\pi E^{1/2}}{\left(m\omega\lambda^2/8\right)^{3/2}}.$$  \hspace{1cm} (8)

and determine the number of doubly occupied sites of a two-component, noninteracting Fermi gas, where both species have the same Fermi distribution function

$$f(E) = \frac{1}{(e^{(E-\mu)/k_BT}+1)^{-1}}$$

according to

$$N_2 = \int_{-\infty}^{\infty} \rho(E) f^2(E) \, dE.$$ \hspace{1cm} (9)

Here the chemical potential \(\mu\) is determined from the normalization to the total particle number

$$N = \int_{-\infty}^{\infty} \rho(E) f(E) \, dE$$

per spin state. In a three-dimensional optical lattice, we use an expansion similar to the Sommerfeld expansion for free electrons \[32\] to obtain the fraction of doubly occupied lattice sites \[33\]

$$n_2 = \frac{N_2}{N} = 1 - \frac{3}{2} \frac{k_B T}{E_F} + \frac{\pi^2}{8} \left(\frac{k_B T}{E_F}\right)^3 + \mathcal{O}\left(\left(\frac{k_B T}{E_F}\right)^4\right).$$ \hspace{1cm} (10)

From our measured value of \(n_2 = 0.43\) we conclude that the temperature of the atoms in the optical lattice is at most \(T/T_F = 0.46\). A similar result for our experimental data was computed numerically in \[8\]. This value gives an upper limit to the temperature since it assumes adiabatic formation of molecules at all doubly occupied sites and a perfect 50:50 mixture of the spin states. Moreover, we have not verified experimentally that the sample in the lattice is indeed in thermal equilibrium. During the ramp across the Feshbach resonance the density distribution might slightly change as compared to the initial noninteracting case, which limits the accuracy of the temperature determination. This principle of thermometry can be also extended to lower potential depth of the optical lattice. For this regime, however, a full numerical calculation of the double occupancy is required.

5. Prospects for interacting fermions in optical lattices

The experiments on Feshbach resonances in optical lattices have already demonstrated the physical richness of interacting Fermi systems. The physics of the Hubbard model can be accessed and studied. Attaining superfluid, Mott insulating and anti-ferromagnetic phases \[2\] will establish optical lattices as a tool for quantum simulations of many-body states. Moreover ‘new physics’ can be expected beyond the single band Hubbard model, a regime which is accessible with Feshbach resonances in optical lattices. Experimental investigations could promote an understanding of this regime since quantitative theoretical predictions are very difficult to obtain.

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