Quantum degenerate atomic gases trapped in the periodic potential of an optical lattice form a quantum many-body system of unprecedented purity. The short-range interaction due to atom-atom collisions makes optical lattices ideal to experimentally realize Hubbard models \[ 1, 2 \]. Experimental studies of bosonic Mott insulators \[ 3, 4, 5, 6 \] and of a fermionic band insulator \[ 7 \] have provided a first taste of this new approach to quantum many-body physics.

In the vicinity of a Feshbach resonance the collisional interaction strength between two atoms is tunable over a wide range. For two fermionic atoms on one lattice site strong interactions change the properties of the system qualitatively and physics beyond the standard Hubbard model becomes accessible. Crossing the Feshbach resonance in one direction leads to an interaction induced coupling between Bloch bands which has been observed experimentally \[ 8 \] and described theoretically \[ 9 \]. Crossing the resonance in the other direction converts fermionic atoms into bosonic molecules. These processes have no counterpart in standard condensed matter systems and demand novel approaches to understand the mixed world of fermions and bosons in optical lattices \[ 3, 10, 11, 12 \]. Descriptions based on multi-band Hubbard models are extremely difficult to handle and therefore the low-tunneling limit is often used as an approximation. In this limit the lattice is considered as an array of microscopic harmonic traps each occupied with two interacting atoms in different spin states.

The harmonic oscillator with two interacting atoms has been studied theoretically and the eigenenergies have been calculated in various approximations \[ 13, 14, 15 \]. Its physics is governed by several length scales. The shortest scale is the characteristic length of the van-der-Waals interaction potential between the atoms. The next larger length scale is given by the s-wave scattering length characterizing low-energy atomic collisions. However, near the Feshbach resonance it may become much larger than the extension of the harmonic oscillator ground state. A precise understanding of the interactions in this elementary model is a prerequisite in order to comprehend the many-body physics occurring in optical lattice systems with resonantly enhanced interactions.

In this paper we study a spin-mixture of fermionic atoms in an optical lattice and their conversion into molecules by means of a Feshbach resonance. The binding energy as a function of the s-wave scattering length between the particles is measured and compared with theoretical predictions. Moreover, we demonstrate that the molecule formation can serve as a measure of the temperature of the atoms in the lattice. For mapping out the phase diagram of many-body quantum states in the lattice the temperature is a key parameter. So far, temperature has not been measured in a lattice since standard methods – such as observing the rounding-off of the Fermi surface – turned out to be dominated by the inhomogeneity of the trapping potential rather than by temperature \[ 16 \]. However, we find that the occupancy of the lattice depends strongly on the temperature \[ 17, 18, 19 \] and the conversion of pairs of atoms into molecules is a sensitive probe, similar to the case of harmonically trapped fermions \[ 20 \].

In a previous experiment, deeply bound molecules of bosonic atoms have been created in an optical lattice by photo-association and were detected by a loss of atoms \[ 21 \]. There the binding energy is only determined by the atomic properties and does not depend on the external potential, nor can the scattering properties between the molecules be adjusted. In low-dimensional systems molecules produced by a Feshbach resonance using fermionic atoms have been observed recently \[ 22, 23 \].

Our experimental procedure used to produce a degenerate Fermi gas has been described in detail in previous work \[ 5 \]. In brief, fermionic \(^{40}\)K atoms are sympathetically cooled by thermal contact with bosonic \(^{87}\)Rb atoms, the latter being subjected to forced microwave evaporation. After reaching quantum degeneracy for both species we remove all rubidium atoms from the trap. The potassium atoms are then transferred from the magnetic trap into a crossed-beam optical dipole trap which consists of two horizontally intersecting laser beams. In the optical trap we prepare a mixture of the \(|F = 9/2, m_F = -9/2\rangle\) and the \(|F = 9/2, m_F = -7/2\rangle\) state with \((50 \pm 4)\%\) in each spin state \[ 24 \] and perform additional evaporative
cooling at a magnetic field of $B = 227 \, G$. At the end of the evaporation we reach temperatures of $T/T_F = 0.25$ with up to $2 \times 10^5$ particles. The temperatures are determined from a fit to the density distribution of the non-interacting atomic cloud after ballistic expansion.

We tune the magnetic field to $B = (210.0 \pm 0.1) \, G$, such that the s-wave scattering length between the two states vanishes. The atoms are then transferred into the optical lattice formed by three orthogonal standing waves with a laser wavelength of $\lambda = 826 \, nm$. The resulting optical potential depth $V_0$ is proportional to the laser intensity and is conveniently expressed in terms of the recoil energy $E_r = \hbar^2 k^2/(2m)$, with $k = 2\pi/\lambda$ and $m$ being the atomic mass.

In the optical lattice we create a band insulator for each of the two fermionic spin states $\uparrow \downarrow$. 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 final value close to the Feshbach resonance located at $B_0 = 202.1 \, G$. From the parameters of our magnetic field ramp we estimate that the molecule formation is performed adiabatically. We measure the binding energy $E_B$ of the dimers by radio-frequency spectroscopy. A pulse with a frequency $\nu_{RF}$ and a duration of $40 \, \mu s$ dissociates the molecules and transfers atoms 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 after dissociation are essentially noninteracting (see fig. 1). We vary the detuning $\delta = \nu_{RF} - \nu_0$ from the resonance frequency $\nu_0$ of the atomic $| -7/2 \rangle \rightarrow | -5/2 \rangle$ transition. The power and duration of the pulse is chosen to constitute approximately a $\pi$-pulse on the free atom transition. The number of atoms in each spin state is determined using absorption imaging after ballistic expansion. For this we ramp down the lattice exponentially with a duration of 1 ms and time constant of 0.5 ms from the initial depth $V_0$ to $5 \, E_r$ to reduce the kinetic energy of the gas and then quickly turn off the trapping potential within a few $\mu s$. The magnetic offset field is switched off at the start of the expansion, so that no molecules can be formed in the short time that it passes the Feshbach resonance. We apply a magnetic field gradient during 3 ms of the total 7 ms of ballistic expansion to spatially separate the spin components.

Figure 1b and c show rf spectra of atoms and molecules trapped in a three-dimensional lattice with a potential depth of $V_0 = 22 \, E_r$, which corresponds to a trapping frequency of $\omega = 2\pi \times 65 \, kHz$ in the potential wells of the lattice. The spectrum in figure 1a is taken at a magnetic field of $B = 202.9 \, G$, corresponding to $a/a_{ho} = -1.3$. We have calculated the ground state radius $a_{ho} = 64 \, nm$ by minimizing the energy of a Gaussian trial wave function inside a single well of our lattice potential. As compared to a Taylor expansion of the sinusoidal potential around the minimum this results in slightly more accurate values. The s-wave scattering length is denoted by $a$. For negative scattering length the molecules are only bound when they are strongly confined whereas no bound state would exist in the homogeneous case. The spectrum exhibits two resonances: the one at $\delta = 0$ corresponds to the atomic transition from the $| -7/2 \rangle$ into the $| -5/2 \rangle$ state. This transition takes place at all lattice sites which initially were only singly occupied and no molecule has been formed. The second resonance at $\delta > 0$ corresponds to the molecular dissociation and is shifted from the atomic resonance by the binding energy. Simultaneous with the increase in the $| -5/2 \rangle$ atom number we observe a loss of atoms in the $| -7/2 \rangle$ state, whereas the $| -9/2 \rangle$ remains unaffected. This is expected since the rampdown of the lattice before detection dissociates all molecules and the $| -9/2 \rangle$ atom number should be fully recovered. Residual fluctuations of the $| -9/2 \rangle$ atom number are probably due to uncertainties in the atom number determination since we do not observe a specific pattern in our spectra.

With the magnetic field tuned to $B = 202.0 \, G$ (see fig.
The scattering length is derived from the magnetic field energy of the molecules on the scattering length (Fig. 2). 

\[ \sqrt{\frac{\Gamma(-E/2\hbar\omega)}{\Gamma(-E/2\hbar\omega - 1/2)} = \frac{\hbar\omega}{a}, } \tag{1} \]

where \( \Gamma(x) \) denotes the Gamma function. We find the normalized binding energy \( E/\hbar\omega \) to be independent of the strength of the lattice and all data points agree well with the theoretical prediction of equation (1) without adjustable parameters. A pseudopotential approximation is valid, as long as \( a_{ho} \) is large compared to the characteristic length scale of the van-der-Waals potential between the two atoms \( \beta_6 = (mC_6/h^2)^{1/4} \) \( \[14\,15\] \), which for our experiments is \( a_{ho}/\beta_6 > 10 \). However, for \( a \gg a_{ho} \) an energy-dependent pseudopotential will model the system more accurately. We have calculated the effective range of the interaction to be \( r_{eff} = 98 a_0 \) \( \[32\] \) and the eigenenergies using an energy-dependent pseudopotential \( \[14\] \) (dashed line in figure 2). Both models agree to within a few percent, 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 \( \[9\,15\] \) and could be tested with our data.

From a quantitative analysis of the spectra we obtain information about the occupancy of our lattice. We measure the ratio between the atomic and the molecular peak heights in the spectra of the \( | - 5/2 \rangle \) atoms and determine the fraction of atoms that where bound in a molecule. Figure 3 shows the measured data for a lattice with a potential depth of 15 \( E_r \). The detected molecular fraction decreases for large values of \( 1/a \), i.e. for deeply bound molecules, because of the small overlap of the initial molecular and the final atomic wave function in the rf transition. From the analytical wave function of the molecular state in relative coordinates \( \psi_{ho}(r) \) \( \[12\] \) we calculate the overlap integral with the harmonic oscillator ground state \( \psi_{ho}(r) = (\pi a_{ho}^2)^{-3/4} \exp(-r^2/2a_{ho}^2) \) which determines the relative strength of the molecular transition assuming that the center-of-mass motion remains unaffected by the rf transition. We fit the overlap integral to our experimental data and obtain the fraction of molecules in the lattice to be \( (43 \pm 5)\% \) (solid line in figure 3).

The observed fraction of molecules is primarily determined by the filling of the lattice. To study the relation between the temperature and filling we have numerically calculated the density of states for noninteracting fermions in an optical lattice including the Gaussian confining potential due to the transverse envelope of the lattice lasers. In the low-tunnelling limit we find that the density of states approaches \( p(E) \propto E^\nu \) with \( \nu = 1/2 \) independent of the lattice depth \( \[18\] \). The fraction of doubly occupied lattice sites in a 50:50 spin mixture depends on \( \nu \) and \( T/T_F \). This makes the molecule fraction a quantity ideally suited for thermometry. Assuming that the occupation probability per spin state and

\[ \left\langle \frac{n}{2} \right\rangle = \frac{1}{\sqrt{\pi}} \frac{\hbar\omega}{a}, \]

We have investigated the dependence of the binding energy of the molecules on the scattering length (Fig. 2). The scattering length is derived from the magnetic field using the parametrization of the Feshbach resonance \( a(B) = a_{ho}(1 - \frac{\Delta B}{B_{ho}}) \), with \( a_{ho} = 174 a_0 \) \( \[30\] \) and \( \Delta B = 7.8 \, G \) \( \[31\] \). We compare our data with the theory for two particles trapped in a harmonic oscillator potential interacting via an energy-independent pseudopotential \( \[13\] \). The binding energy \( E \) of the molecules depends on the scattering length according to

\[ \frac{\Gamma(-E/2\hbar\omega)}{\Gamma(-E/2\hbar\omega - 1/2)} = \frac{\hbar\omega}{a}. \]
lattice site $i$ is $0 < n_i < 1$, the probability of finding two atoms with different spin state on a lattice site is $n_i^2$. We identify the molecule fraction with the mean value of $n_i^2$ over the whole lattice. From a comparison with a numerical calculation \[18\] we can conclude that the temperature of the atoms in the optical lattice is at most $T / T_F = 0.45 \pm 0.03$. A similar result for our experimental parameters was computed in \[15\]. 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. 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.

We measure the lifetime of the molecules in the lattice to be on the same order of magnitude as of molecules in an optical dipole trap \[31\]. This is probably related to the tunnelling rate, which for our lattice parameters is on the order of 100 Hz and therefore the rate of three-body collisions is comparable to the optical trap. We expect that the lifetime of the molecules will significantly increase if the lattice depth becomes larger than 30 $E_r$. Another possible mechanism which could lead to a loss of molecules is photo-association induced by the lattice laser beams.

In conclusion, we have studied molecules in a three-dimensional optical lattice. We have measured the binding energies and find good agreement with the fundamental theoretical model of two interacting particles in a harmonic potential well. Moreover, we have measured the filling of the lattice by determining the fraction of molecules formed. This allows for thermometry in the lattice, which has previously been unaccessible. The fraction of created molecules gives direct access to the number of doubly occupied lattice sites in a two-component Fermi gas. Therefore it could be employed to characterize a Mott insulating phase where the double occupancy should be strongly reduced.

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\[\text{FIG. 3: The fraction of molecules detected by rf-spectroscopy at a potential depth of } 15 E_r. \text{ For weakly bound molecules } (a_{ho}/a < -1) \text{ the dissociation works well since the overlap between the molecular and the atomic wave function is large. For deeply bound molecules } a_{ho}/a > 0 \text{ the detected molecular fraction is suppressed due to the vanishing overlap between the wave functions. The solid line shows the theoretical expectation for a constant molecular fraction of 43\%.} \]
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