P H Y S I C A L R E V I E W L E T T E R S

Molecules of Fermionic Atoms in an Optical Lattice

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We create molecules from fermionic atoms in a three-dimensional optical lattice using a Feshbach resonance. In the limit of low tunneling, the individual wells can be regarded as independent three-dimensional harmonic oscillators. The measured binding energies for varying scattering length agree excellently with the theoretical prediction for two interacting atoms in a harmonic oscillator. We demonstrate that the formation of molecules can be used to measure the occupancy of the lattice and perform thermometry.

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 [3–6] 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 [7] and described theoretically [8]. 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 [9–12]. Descriptions based on multiband 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 [9,13–16]. 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 phys-

ics occurring in optical lattice systems with resonantly enhanced interactions.

In this Letter 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 [17–19] 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 photoassociation and were detected by a loss of atoms [6,21]. There the binding energy is determined only 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 [7]. 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

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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 2×10^5 particles. The temperatures are determined from a fit to the density distribution of the noninteracting 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 [7]. 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 [7]. 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 [25]. 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 [23,26,27]. A pulse with a frequency ν_{rf} and a duration of 40 μs 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(a)]. We vary the detuning $\delta = \nu_{rf} - \nu_0$ from the resonance frequency ν_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 π 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 a time constant of 0.5 ms from the initial depth V_0 to $5E_r$ to reduce the kinetic energy of the gas, and then quickly turn off the trapping potential within a few μs. 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.

Figures 1(b) and 1(c) show rf spectra of atoms and molecules trapped in a three-dimensional lattice with a potential depth of $V_0 = 22E_r$, which corresponds to a trapping frequency of $\omega = 2\pi \times 65$ kHz in the potential wells of the lattice. The spectrum in Fig. 1(b) 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
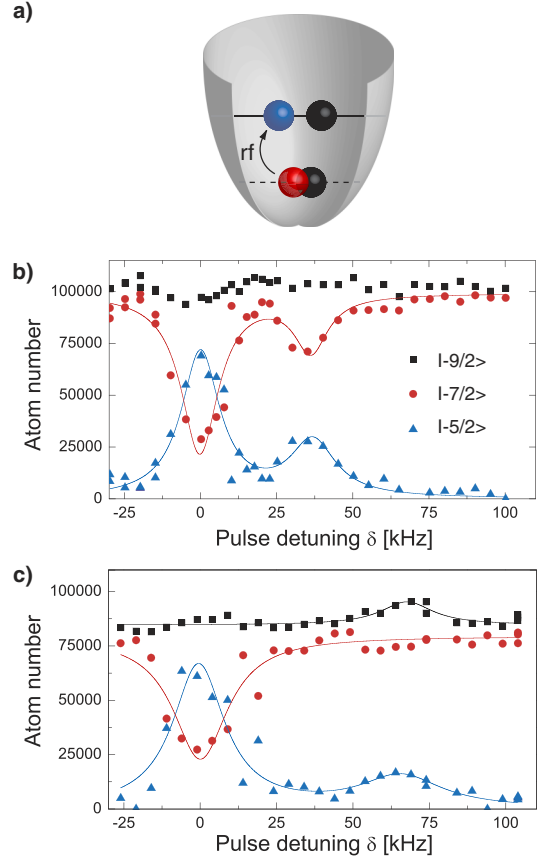

FIG. 1 (color online).   (a) Illustration of the rf spectroscopy between two bound states within a single well of the optical lattice. The atoms in the initial states $|-7/2\rangle$ and $|-9/2\rangle$ are converted into a bound dimer by sweeping across a Feshbach resonance. Subsequently we drive an rf transition $|-7/2\rangle \rightarrow |-5/2\rangle$ to dissociate the molecule. (b) rf spectrum taken at $B = 202.9$ G, i.e., for $a < 0$. (c) rf spectrum taken at $B = 202.0$ G, i.e., for $a > 0$. All data are taken for a lattice depth of $22E_r$. The lines are Lorentzian fits to the data.

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 bound only 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 where no molecule has been formed. The second resonance at $\delta > 0$ corresponds to 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 ramp-down 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 numbers are probably due to uncertainties in the atom number determination since we do not observe a reproducible pattern in our spectra.

With the magnetic field tuned to $B = 202.0$ G [see Fig. 1(c)], which corresponds to $a/a_{ho} = 16.8$, the spectrum changes qualitatively. For this value of the scattering length stable molecules exist even in free space, but the molecules formed in the lattice are not detected by our state-selective imaging procedure unless they are dissociated by the rf pulse. Therefore only rf dissociated atom pairs show up in the time-of-flight images, resulting in an increasing number of atoms in the $|-5/2\rangle$ and the $|-9/2\rangle$ state at the molecular resonance.

In contrast to earlier work, where molecules were dissociated into a continuum and the fragments were essentially free particles [23,26,27], the fragments in our configuration occupy an energy eigenstate of the confining potential. In such a bound-bound transition no extra kinetic energy is imparted onto the dissociated fragments since any excess excitation energy would have to match the band gap. 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 [28,29] 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 (Fig. 2). The scattering length is derived from the magnetic field using the parametrization of the Feshbach resonance $a(B) = a_{bg}(1 - \frac{\Delta B}{B - B_0})$, with $a_{bg} = 174a_0$ [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

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

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 Eq. (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 $\beta_6 = (mC_6/\hbar^2)^{1/4}$ [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 $r_{eff} = 98a_0$ [32] and the eigenenergies using an energy-dependent pseudopotential [14] (dashed lines in Fig. 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 mea-
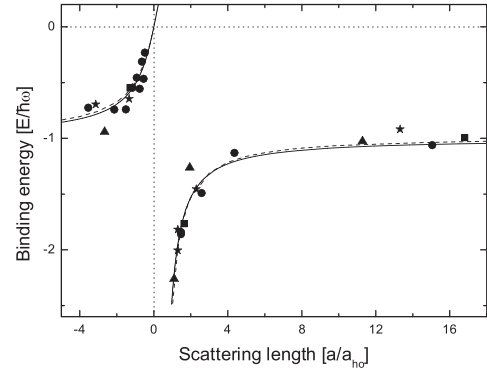

FIG. 2. The measured binding energy of molecules in a three-dimensional optical lattice. The data are taken for several potential depths of the optical lattice of $6E_r$ (triangles), $10E_r$ (stars), $15E_r$ (circles), and $22E_r$ (squares). The solid lines correspond to the theory of Ref. [13] with no free parameters; the dashed lines use an energy-dependent pseudopotential according to Ref. [14]. At the position of the Feshbach resonance ($a \to \pm\infty$) the binding energy takes the value $E = -\hbar\omega$.

sure 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 $15E_r$. 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 $\psi_m(\mathbf{r})$ [13], we calculate the overlap integral with the harmonic oscillator ground state $\psi_{ho}(\mathbf{r}) = (\pi a_{ho}^2)^{-3/4}\exp(-\mathbf{r}^2/2a_{ho}^2)$ which determines the relative strength of the molecular transition assuming that the center-of-mass motion remains unaf-
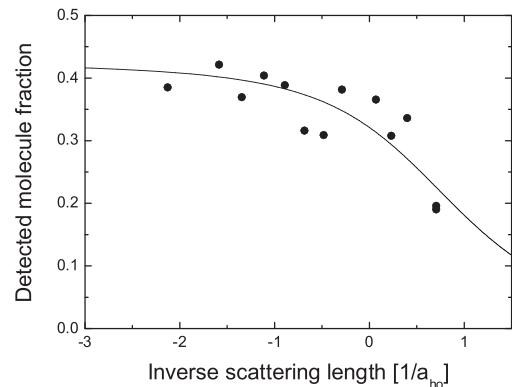

FIG. 3. The fraction of molecules detected by rf spectroscopy at a potential depth of $15E_r$. For weakly bound molecules ($a_{ho}/a < -1$) the dissociation works well since the overlap between the molecular and the atomic wave functions is large. For deeply bound molecules $a_{ho}/a > 0$ the detected 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%.

fected 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 Fig. 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-tunneling limit, we find that the density of states approaches $\rho(E) \propto E^{\nu}$, 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 ν and T/T_F. This makes the molecule fraction a quantity ideally suited for thermometry. Assuming that the occupation probability per spin state and 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 [17]. 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 tunneling 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 $30E_r$. Another possible mechanism which could lead to a loss of molecules is photoassociation 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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