Tuning a Feshbach Resonance through a Shape Resonance in the Dissociation of Ultracold Molecules

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We study the dissociation of ultracold molecules made from an atomic Bose-Einstein condensate using a Feshbach resonance with a d-wave bound state. The dissociation populates two partial waves, thus creating a spatial interference pattern. One of the partial waves exhibits a shape resonance, which is studied by tuning the Feshbach resonance through it. A theory for the dissociation is developed and agrees well with the experiment.

Shape resonances and Feshbach resonances are observed in scattering experiments in many fields of physics. A shape resonance is caused by a quasi-bound state behind a potential barrier, such as the centrifugal barrier, whereas a Feshbach resonance is caused by a (quasi)-bound state in another collision channel, such as a channel with different spin configuration. So far, it was not possible to tune one scattering resonance through another. We now performed such an experiment with ultracold molecules made from an atomic Bose-Einstein condensate. Instead of performing a standard scattering experiment, we capture the same physics in a dissociation experiment, with the population initially prepared in the molecular state. The population decays into two partial waves of unbound atom pairs, thus creating a spatial interference pattern. The relative phase between the partial waves, the branching ratio, and the total decay rate display a clear signature of a shape resonance.

In the field of ultracold atomic gases, the energy of the (quasi)-bound molecular state that causes the Feshbach resonance (the "Feshbach state") can be tuned with a magnetic field. This makes it possible to transfer long-lived population into this state by starting from an atomic Bose-Einstein condensate (BEC) and then ramping the magnetic field slowly across B_{res}, the position of the zero-energy Feshbach resonance [1–8]. With a ramp towards lower fields, the Feshbach state becomes truly bound, so that the bound atom pairs form actual molecules.

The molecules can be dissociated by ramping the magnetic field back through B_{res}. At the final magnetic field, the Feshbach state is only quasi-bound and the population decays rapidly into unbound atom pairs. The decay rate and the energy of the dissociated atoms can be tuned by varying the final magnetic field. Previous experiments that investigated this dissociation [9, 10] worked with Feshbach resonances involving s-wave (quasi)-bound states or low energies, so that the dissociation populated only the atomic s wave. In this paper, the molecule dissociation is investigated for a Feshbach resonance with a d-wave (quasi)-bound state. This state dissociates into atomic s and d waves, thus creating a spatial interference pattern between the two partial waves. The dissociation process is particularly interesting in ^{87}Rb, because this isotope features a d-wave shape resonance. It thus becomes possible to tune a Feshbach resonance through a shape resonance.

The d-wave shape resonance in ^{87}Rb is caused by the highest-lying d-wave bound state in the open channel (the "shape-resonance state"). This state is only quasi-bound, because it lies *above* the open-channel threshold. The state is localized behind the centrifugal barrier and population in it decays spontaneously with a mean life of ~ 60 ns into unbound d-wave atom pairs by tunnelling through the centrifugal barrier. This state was first observed in a photoassociation experiment [11]. Very recently, a scattering experiment showing the effect on the cross-section near $B = 0$ was carried out by two groups independently [12, 13].

Obviously, the shape-resonance state drastically affects the decay of the Feshbach state when the magnetic field is chosen such that the energies of the two states match. Population is then resonantly transferred from the Feshbach state to the shape-resonance state and subsequently decays quickly into unbound d-wave atom pairs by tunnelling through the centrifugal barrier, thus substantially increasing the decay rate of the Feshbach state.

The experimental set-up was described in detail elsewhere [3, 10, 14]. In brief, a BEC of ^{87}Rb atoms in the hyperfine state $|f, m_f\rangle = |1, 1\rangle$ is released from an optical dipole trap. One millisecond after the release, population is transferred into the Feshbach state by slowly ramping the magnetic field across a Feshbach resonance near 632 G [14], which has a width of 1.3 mG [10]. Since $B < B_{res}$ after the ramp, the molecules are stable. Remaining atoms are spatially separated from the molecules with a Stern-Gerlach field. This crucial step removes all incoming atom flux from the spatial region of inter-
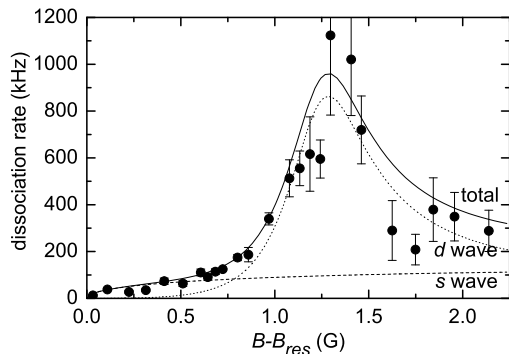
FIG. 1: Molecule dissociation rate Γ as a function of magnetic field B with respect to the position of the zero-energy Feshbach resonance B_{res}. The experimental data for the total rate (circles) clearly show the effect of the d-wave shape resonance near 1.2 G. The solid line shows the prediction from our theoretical model for the total dissociation rate and agrees well with the data. The dashed and dotted lines show the predicted partial dissociation rates into the s and d waves, respectively.

est. The magnetic field is then ramped to a fixed value $B_{hold} > B_{res}$ as fast as possible ($dB/dt \approx 1$ G/μs) and then held there for a time t_{hold}. Experimentally, the kink in B at the beginning of t_{hold} has a settling time of ~ 1 μs. During t_{hold}, population in the Feshbach state decays exponentially with a mean life $1/\Gamma(B)$. After t_{hold}, the magnetic field is switched off rapidly and after 0.85 ms time of flight (counting from the dissociation) an absorption image is taken. Molecules that did not decay during t_{hold} are invisible in the image, because only unbound atoms resonantly absorb light from the detection laser beam.

The total dissociation rate $\Gamma(B)$ is extracted from a series of images for fixed B_{hold} and variable t_{hold}. The total number of dissociated atoms is determined from each image and then fit to an exponential decay as a function of t_{hold}. This yields the total dissociation rate shown in Fig. 1. The enhanced decay rate near 1.2 G due to the d-wave shape resonance is clearly visible. The low magnetic-field data agree well with theory. Measurements for magnetic fields near the shape resonance are difficult, because the large decay rates require extremely fast magnetic-field control. Measurements for magnetic fields above the shape resonance suffer from loss of signal during the two passages through the shape resonance at the beginning and the end of t_{hold}.

Typical absorption images are shown in Fig. 2. The images show a spatial interference pattern created by the two partial waves, which have quantum numbers $(l, m_l) = (0, 0)$ and $(2, 0)$ for the rotation of the atoms around each other [15]. Similar interference patterns have recently been seen in Refs. [12, 13]. The interference pattern can be phenomenologically described by the follow-
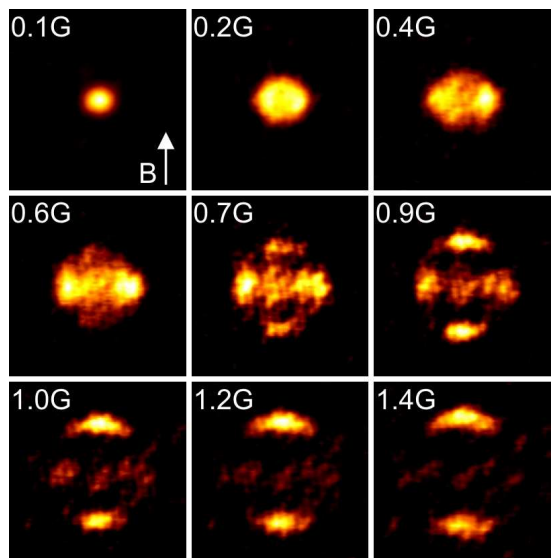

FIG. 2: Time-of-flight images of unbound atoms obtained in the molecule dissociation. The images were taken at different values of $B - B_{res}$. The magnetic field is vertical in the images. The interference between the s and d partial wave undergoes a change in relative phase and amplitude. At 0.1 G, the dissociation is mostly s wave, producing a circle. For higher magnetic fields, both partial waves are populated. From 0.2 to 0.6 G, the interference suppresses atom emission *along* B, whereas the opposite relative phase in the interference between 1.0 and 1.4 G suppresses emission *perpendicular* to B. At 0.7 and 0.9 G, the relative phase is such that neither component is strongly suppressed. The typical radius reached by the atoms during the constant time of flight increases for increasing B, thus indicating an increase of the kinetic energy released in the dissociation.

ing wave function

$$\psi_{decay}(\vec{r}) = g(r, t) \left(e^{i\delta_0} \sqrt{\beta_0} Y_{00} - e^{i\delta_2} \sqrt{\beta_2} Y_{20}(\vartheta) \right) \quad (1)$$

where $Y_{lm}(\vartheta, \varphi)$ is a spherical harmonic, δ_l and β_l characterize the phase and amplitude of the partial waves, and $g(r, t)$ is some radial wave function that is of little relevance here. The normalization of $g(r, t)$ is chosen such that $\beta_0 + \beta_2 = 1$, which implies that β_l is the branching ratio for decay into the l-th partial wave.

The branching ratio β_2 and the relative phase $\delta_2 - \delta_0$ are extracted from the images with the same method as used in Ref. [13]. In brief, computerized tomography is used to reconstruct the 3-dimensional (3D) density distribution from the 2D images. The 3D density is sorted into 20 bins to obtain the probability $W(\vartheta)$ for finding an atom at angle ϑ. A fit of the angular part of the modulus squared of Eq. (1) to $W(\vartheta)$ yields the fit parameters β_2 and $\delta_2 - \delta_0$. These parameters are shown in Fig. 3. The branching ratio clearly shows the enhanced decay into the d wave due to the shape resonance. The d-wave phase shows a positive phase shift of almost π shaped like an inverse tangent, which is typical of a shape reso-
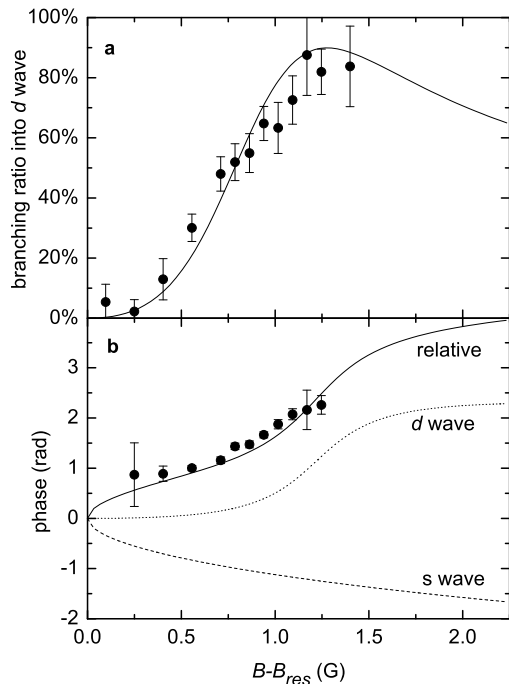
FIG. 3: Parameters extracted from the spatial interference patterns. (a) Branching ratio for decay into the d wave. Again, the shape resonance is clearly visible. The experimental data (circles) agree well with the theory (line). (b) Partial-wave phases and relative phase. The solid, dashed, and dotted lines show the theoretical prediction for the relative phase $\delta_2 - \delta_0$, the s-wave phase δ_0, and the d-wave phase δ_2, respectively. The phase shift of almost π in δ_2 is typical of a shape resonance. Experimental data (circles) match the solid line well.

nance. In regions where the branching ratio is close to 0 or 1, the fit cannot reliably determine the relative phase. The position of the shape resonance is usually defined as the position of the inflection point of the d-wave phase in Fig. 3b, which lies at 1.22 G.

In order to analyze the decay quantitatively, we performed a coupled-channels calculation for a scattering *gedanken* experiment that is closely related to the dissociation experiment performed here. In the *gedanken* experiment, we consider a colliding atom pair with kinetic energy E in the relative motion in the presence of a magnetic field B near the 632 G Feshbach resonance. S-matrix elements $S_{ll'}$ are calculated in the E-B-plane for l and l' equal to 0 or 2 (both with $m_l = 0$). According to the theory of multichannel scattering resonances, these S-matrix elements are expected to follow an analytic expression of the form [16, 17]

$$S_{ll'}(E,B) = \left(\delta_{ll'} - \frac{i\hbar\Gamma_{ll'}(E)}{E - E_F(B) + \frac{i}{2}\hbar\Gamma(E)} \right) \times e^{i[\delta_l(E)+\delta_{l'}(E)]} . \quad (2)$$

Here, $\delta_{ll'}$ is the Kronecker symbol, $\Gamma(E)$ is the total decay rate of the Feshbach state, $E_F(B)$ is the energy of the Feshbach resonance with respect to the open-channel threshold (including a small shift that is of little relevance here), and the significance of the partial-decay-rate parameters $\Gamma_{ll'}(E)$ will be discussed below. Finally, $\delta_l(E)$ is the background scattering phase for the l-th partial wave, where background means for magnetic fields far away from the Feshbach resonance. Restricting our considerations to a small range of magnetic fields, the magnetic-field dependence of E_F is approximately linear

$$E_F(B) = (B - B_{res})\Delta\mu , \quad (3)$$

where B_{res} is the position of the zero-energy Feshbach resonance, and $\Delta\mu$ is the difference of the magnetic moments between a closed-channel molecule and an open-channel atom pair.

For the S-matrix to be unitary and symmetric, the parameters $\Gamma_{ll'}(E)$ must all be real and fulfill $\Gamma_{00} + \Gamma_{22} = \Gamma$ and $\Gamma_{20} = \Gamma_{02} = \pm\sqrt{\Gamma_{00}\Gamma_{22}}$. We find from our coupled-channels calculation that in our case $\Gamma_{20} = \Gamma_{02} = -\sqrt{\Gamma_{00}\Gamma_{22}}$. For any given E, we fit Eq.(2) for variable B to the S-matrix elements obtained from our coupled-channels calculation. The fits match the S-matrix extremely well. The open-channel physics, including the shape resonance, is independent of B and is therefore fully included in the energy-dependent fit parameters $\delta_l(E)$, $\Gamma(E)$, and $\Gamma_{ll'}(E)$. Furthermore, the combination of the fits yields $B_{res} = 632.3$ G and $\Delta\mu = 2\pi\hbar \times 4.67$ MHz/G.

We will now discuss the connection between the dissociation experiment presented in this paper and the energy-dependent fit parameters $\delta_l(E)$, $\Gamma(E)$, and $\Gamma_{ll'}(E)$. First of all, the kinetic energy E of the atom pairs after dissociation is related to B through the simple relation $E = E_F(B)$, because energy is conserved in the dissociation process. Therefore the energy-dependent fit-parameters for the *gedanken* experiment become magnetic-field dependent parameters in the dissociation experiment. In the context of the dissociation experiment, we therefore call them $\delta_l(B)$, $\Gamma(B)$, and $\Gamma_{ll'}(B)$.

The link between the scattering *gedanken* experiment and the dissociation experiment can be established from evaluating the different terms in the asymptotic form of the regular scattering wave function

$$\psi^{(+)}(\vec{r}) \stackrel{r\to\infty}{\longrightarrow} (-1)^{l'} \frac{e^{-ikr}}{r} Y_{l'0}(\vartheta)$$
$$- \frac{e^{ikr}}{r} \sum_l \left(S_{ll'}^{bg} + S_{ll'}^{res} \right) Y_{l0}(\vartheta) , \quad (4)$$

where we assume in the *gedanken* experiment that only one partial wave l' is initially populated. Here, k is related to the energy by $E = \hbar^2 k^2 / (2m_{red})$ with the reduced mass m_{red}, and we split the S-matrix into a back-

ground part and a resonant part $S_{ll'} = S_{ll'}^{bg} + S_{ll'}^{res}$ with $S_{ll'}^{bg} = e^{2i\delta_l(E)}\delta_{ll'}$.

The scattering wave function consists of three parts: an incoming wave, an outgoing background wave, and an outgoing resonant wave. The resonant part is due to particles that make the transition to the Feshbach state and subsequently decay back into the open channel. The Stern-Gerlach separation removes all incoming flux and along with it the background scattered wave. Hence, these two terms need to be removed from the scattering state in order to describe the decay wave function

$$\psi_{decay}(\vec{r}) \xrightarrow{r\to\infty} -\frac{e^{ikr}}{r}\sum_l S_{ll'}^{res}Y_{l0}(\vartheta) . \qquad (5)$$

Using the above equations, this can be rewritten to yield Eq. (1), where the branching ratio for decay into the l-th partial wave is given by

$$\beta_l(B) = \frac{\Gamma_{ll}(B)}{\Gamma(B)} . \qquad (6)$$

This means that $\Gamma_{ll}(B)$ represents the partial decay rate into the l-th partial wave. In addition, the phases of the decaying partial waves are identical to the background scattering phases $\delta_l(B)$. The good agreement between theory and experiment without any free fit parameters to adjust them to each other supports the theory developed here.

In conclusion, we showed that a Feshbach resonance can be tuned through a shape resonance in a dissociation experiment. We developed a model that links the dissociation experiment to a scattering experiment. The predictions from this model agree well with the experimental results.

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[15] The association and dissociation of the molecules is due to the spin-spin interaction, which can change l by 0 or ± 2 and conserves $m_{f1} + m_{f2} + m_l$, where m_{f1} and m_{f2} are the magnetic hyperfine quantum numbers of the two atoms. When associating the molecules, the incoming atoms are initially in an s wave, implying $m_l = 0$. Since the entrance channel of the association and the exit channel of the dissociation are identical, m_l must also vanish after the dissociation. The d-wave Feshbach state can therefore dissociate into $(l, m_l) = (0, 0)$, $(2, 0)$, or $(4, 0)$, but the g wave is negligible for the parameters of the present experiment.

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