Very high precision bound state spectroscopy near a ^{85}Rb Feshbach resonance

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We precisely measured the binding energy ($\epsilon_{\rm bind}$) of a molecular state near the Feshbach resonance in a ^{85}Rb Bose-Einstein condensate (BEC). Rapid magnetic field pulses induced coherent atom-molecule oscillations in the BEC. We measured the oscillation frequency as a function of B-field and fit the data to a coupled-channels model. Our analysis constrained the Feshbach resonance position [155.041(18) G], width [10.71(2) G], and background scattering length [-443(3) a$_0$] and yielded new values for v_{DS}, v_{DT}, and C_6. These results improved our estimate for the stability condition of an attractive BEC. We also found evidence for a mean-field shift to $\epsilon_{\rm bind}$.

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The phenomenon of a Feshbach resonance in ultracold collisions of alkali atoms has received much theoretical and experimental interest in recent years and has sparked interest in the subject of resonant Bose-Einstein condensates (BEC). Feshbach resonances [1, 2] have been used to control elastic and inelastic collisions in ultracold gases [3, 4, 5, 6] and for tuning the self-interaction in BEC [7, 8, 9, 10, 11] by changing the magnitude of an external magnetic field. The magnetic field controls the self-interaction in the BEC by affecting the s-wave scattering length, a. Close to resonance, the scattering length varies with B-field according to

$$a = a_{\rm bg}\left(1 - \frac{\Delta}{B - B_{\rm peak}}\right), \qquad (1)$$

where B$_{\rm peak}$ is the resonance position and is defined to be the magnetic field where the magnitude of a becomes infinite, $a_{\rm bg}$ is the background scattering length, and $\Delta = B_{\rm zero} - B_{\rm peak}$ is the resonance width where $B_{\rm zero}$ is the B-field where the scattering length crosses zero. Measurements of Feshbach resonance positions and widths have been used in a variety of alkali atoms to improve the determination of the interatomic potentials. These potentials have then been used to precisely calculate a multitude of important properties for trapped atomic gases [4, 6, 12, 13, 14, 15].

Recently, we applied rapid magnetic field variations near a Feshbach resonance to create an atom-molecule superposition state in a ^{85}Rb BEC [16], which has allowed us to precisely determine the Feshbach resonance position and width. Our novel technique for studying the Feshbach resonance relies on the presence of atom-molecule coherence [17, 18, 19]. By inducing periodic oscillations in the number of condensate atoms, we obtain a direct, high precision measurement of the molecular bound state energy. Exploiting the resonance, we tune the molecular state very close to threshold — to our knowledge, this is the most weakly bound state ever observed. The present method for studying the Feshbach resonance through atom-molecule oscillations offers all of the many inherent advantages of a frequency measurement, including the possibility of high measurement precision, a lack of sensitivity to errors in the absolute atom number calibration, and a simple interpretation of the oscillation frequency in terms of the relative energy difference between the atomic and molecular states. When these advantages are combined with an improved method for magnetic field calibration [20], the present technique for probing the Feshbach resonance is much more precise than previous experiments that examined such Feshbach resonance observables as variable rethermalization rates in a trapped cloud of atoms [4, 14], enhancements of photoassociation rates [3] and inelastic loss rates near the resonance [21], and variations of the mean-field expansion energy of a BEC [7].

To complete our precise characterization of the Feshbach resonance, we also made an improved measurement of B$_{\rm zero}$, the magnetic field where the scattering length vanishes. This experiment is very similar to our previous work [14, 22], where we determined the a=0 field by measuring the critical number (N$_{\rm crit}$) for collapse of a BEC, and then we extrapolated to the magnetic field where N$_{\rm crit}$ would be infinite. We have improved the measurement precision by about a factor of 4 by improving our magnetic field calibration and using a larger number of condensate atoms to measure the collapse. We find B$_{\rm zero}$=165.750(13) G.

The procedure used to generate atom-molecule oscillations in ^{85}Rb Bose-Einstein condensates has been described in previous work [16], so we merely outline the method here. After creating condensates with initial number of atoms N$_0$ $\simeq$16000 at a magnetic field B$\simeq$162 G, we apply two short B-field pulses ($\sim$40 μs duration) that approach and then recede from the Feshbach resonance at B$_{\rm peak}$ $\simeq$155 G. The intermediate value of magnetic field between the pulses, B$_{\rm evolve}$, and the time spacing between pulses, t$_{\rm evolve}$, are variable quantities. The double pulse sequence is followed by a slow change in the B-field to expand the BEC [9], then the trap is switched off (B$\rightarrow$0) and destructive absorption imaging is used to count the number of atoms remaining in the condensate.

As in Ref. [16], periodic oscillations in the BEC number were observed as a function of t_{evolve} (see Fig. 1). We fit the BEC number oscillation to a damped harmonic oscillator function with an additional linear loss term:

$$N(t) = N_{avg} - \alpha t + A \exp\left(-\beta t\right) \sin\left(\omega_e t + \phi\right), \qquad (2)$$

where N_{avg} is the average number, A is the oscillation amplitude, α and β are the number loss and damping rates, respectively, and $\omega_e = 2\pi\sqrt{\nu_0^2 - [\beta/(2\pi)]^2}$. The quantity of interest here is ν_0, the natural oscillator frequency corresponding to the molecular binding energy, ν_0=$\epsilon_{\mathrm{bind}}/h$. We measured the oscillation frequency for values of B_{evolve} from 156.1 G to 161.8 G. Over this range, the frequency varies by over 2 orders of magnitude (10-1000 kHz), but the linear loss rate changes very little. The damping rate shows a significant B-field dependence, increasing from $\beta \simeq 2\pi$ x 0.8 kHz near 156 G to $\beta \simeq 2\pi$ x 22 kHz near 162 G. We find no significant density dependence to the damping at B_{evolve}=158.60(5) G; increasing the total atom density by a factor of 4.3(5) leads to a damping rate increase of only a factor of 1.3(3). Atom loss from the BEC is well described by a linear rate of -2 to -7 atoms/μs over the field range of interest. The rate is consistent with previous measurements of number loss due to a single B-field pulse toward the Feshbach resonance [20].

To characterize the Feshbach resonance, it is necessary to know both the oscillation frequency and B_{evolve}. We precisely measured B_{evolve} by transferring atoms to an untrapped spin state by driving Δm=+1 spin flip transitions with an applied pulse of rf radiation (pulse length=5→25 μs). The spin flip frequency was determined from the rf lineshape for the loss of atoms from the magnetic trap. After measuring the rf transition frequency, we inverted the Breit-Rabi equation to obtain the corresponding B-field. To ensure that the magnetic field was sufficiently constant during t_{evolve}, we mapped out $B(t)$ using rf pulses with lengths short compared to t_{evolve}. Due to interference of the rf radiation with the magnetic field control circuitry, there was a small systematic shift of the field as a function of the rf power used. The uncertainty for each magnetic field determination was the quadrature sum of the uncertainty due to the lineshape measurements (~15 mG) and the uncertainty in the extrapolation to zero rf power (~20 mG). Typically, the total uncertainty in the average B-field was ~25 mG.

The measured oscillation frequencies versus magnetic field are plotted in Fig. 2. We use these data and the zero-crossing field B_{zero} to completely characterize the scattering length and binding energy as a function of magnetic field near the Feshbach resonance. As a starting point we use the coupled-channels analysis of van Kempen et al. [15], where several high-precision data for ^{85}Rb and ^{87}Rb were combined to perform an inter-isotope determination of the rubidium interactions with unprecedented accuracy. The predictive power of this analysis can be seen from Ref. [16], where the initial data on the atom-molecule coherence were already in good agreement with the predicted binding energy of the underlying Feshbach state. Another example of the accuracy of the analysis in Ref. [15] is its agreement with more than 40 Feshbach resonances recently discovered in ^{87}Rb [23].

Van Kempen et al. used the best known values [14] for the resonant magnetic field B_{peak} and zero crossing B_{zero}. In this Letter, we ignore the relatively imprecise value of B_{peak} from Ref. [14], and instead use the measured dependence of binding energy on magnetic field along with the new B_{zero} measurement given above to determine the interaction parameters. We observe that

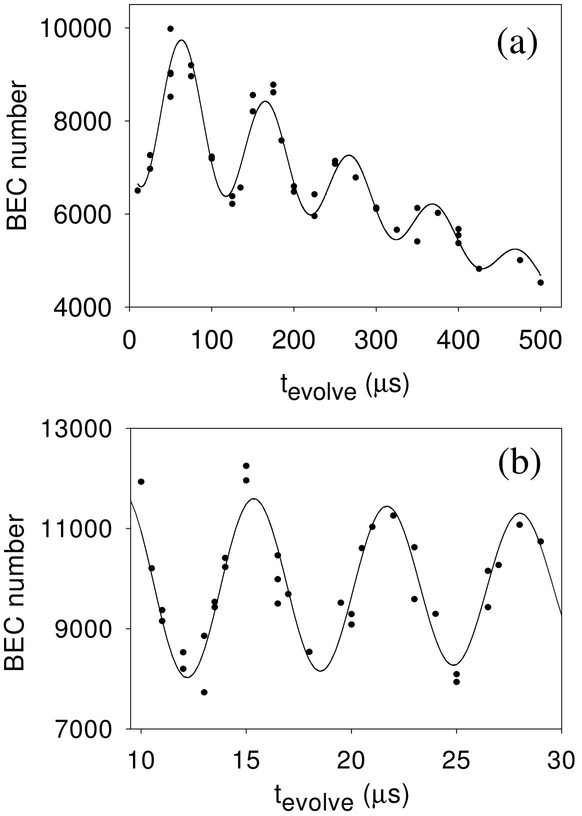

FIG. 1: BEC number versus pulse spacing, t_{evolve}. (a) B_{evolve}=156.840(25) G. At this magnetic field, which is relatively close to resonance, the oscillation frequency is very low (ν_0=9.77(12) kHz) so that the damping and atom loss significantly affect the observed time dependence (here β=2π × 0.58(12) kHz and α=7.9(4) atoms/μs). (b) B_{evolve}=159.527(19) G. Farther from resonance, the time dependence of the BEC number is dominated by the higher oscillation frequency of ν_0=157.8(17) kHz. Damping of the oscillations and atom loss are negligible in the relatively short time window used to determine ν_0.

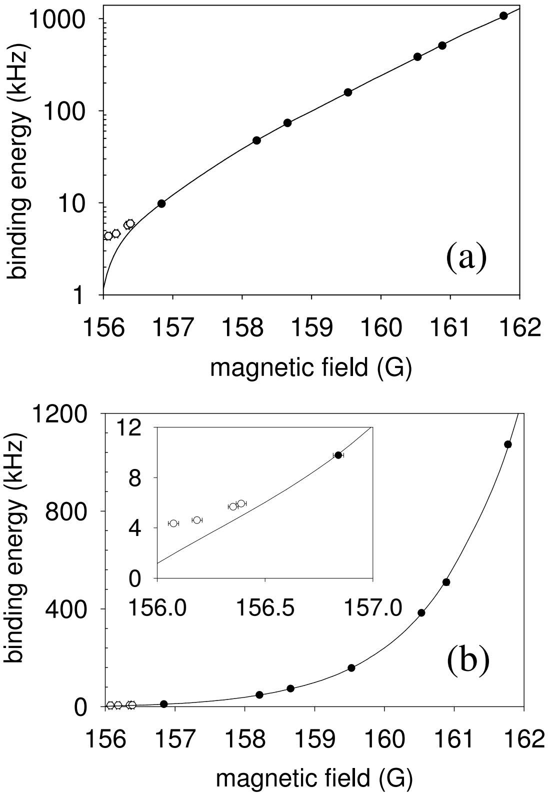

FIG. 2: Molecular binding energy versus magnetic field, B_{evolve}. (a) The points are measured values of the atom-molecule oscillation frequency, ν_0, while the solid line represents the molecular binding energy, which we fit to the data by adjusting the parameters of a coupled-channels scattering theory. Only black points were included in the fit; white points were excluded because they experienced a statistically significant mean-field shift. To improve visibility, the points are larger than the error bars. (b) Same as in (a), but with a linear scale for the vertical axis. The inset shows the deviation of the lowest frequency data from the fit to the rest of the data.

the fitting procedure is mainly sensitive to only three parameters: the van der Waals dispersion coefficient, C_6, and the non-integral vibrational quantum numbers at dissociation, v_{DS} and v_{DT}, which determine the position of the last bound state in the singlet and triplet potentials, respectively. Varying the additional parameters C_8, C_{10}, ϕ_T^E (the first-order energy-dependence of the phase of the oscillating triplet radial wave function), and J, the strength of the exchange interaction, does not improve the fitting because these changes can be absorbed in small shifts of v_{DS}, v_{DT}, and C_6. Therefore, we take the mean values for these four parameters [24] from the most recent determination in Ref. [23].

The best fit to B_{zero} and the seven highest frequency data points yields a reduced χ^2=0.30 for 5 degrees of freedom. This value of χ^2 is improbably low due to the fact that the uncertainty in the data is dominated by the systematic uncertainty in magnetic field related to the magnitude of the rf power shift. Figure 2 shows the theoretical fit to the binding energy data as a function of magnetic field. From the fit, we find substantially improved values for the Feshbach resonance position B_{peak}=155.041(18) G, width Δ=10.71(2) G, and background scattering length a_{bg}=-443(3) a_0. These results may be compared to previously obtained results B_{peak}=154.9(4) G and Δ=11.0(4) G [14], and a_{bg}=-450(3) a_0 [25]. Our best interaction parameter values are C_6=4707(2) a.u., v_{DS}=0.00918(17), and v_{DT}=0.94659(29). Here the error bars do not include systematic errors due to the uncertainties in other interaction parameters that are not constrained by our data. To compare our values with those of Ref. [15], we determined the sensitivity of our three interaction parameters to systematic shifts in the other parameters, as shown in Table I. Using the fractional uncertainties in C_8, C_{10}, ϕ_T^E, and J from Ref. [15], we find C_6=4707(13) a.u., v_{DS}=0.0092(4), and v_{DT}=0.9466(5). All of these values agree with those given in Ref. [15]: C_6=4703(9) a.u., v_{DS}=0.009(1), and v_{DT}=0.9471(2). Our value for v_{DS} is more precise than that of Ref. [15], while v_{DT} and C_6 are slightly less precise. If future experiments allow improvements to the other interaction parameters, then our results will also become more precise since the systematic errors are comparable to or larger than our statistical errors from the fit.

TABLE I: Sensitivities of the determined interaction parameters v_{DS}, v_{DT} and C_6 to fractional uncertainties in C_8, C_{10}, ϕ_T^E and J. For instance, the systematic error in C_6 due to a 10% uncertainty in C_8 is $123 \times 0.10 = 12.3$ a.u.

	$\Delta C_8/C_8$	$\Delta C_{10}/C_{10}$	$\Delta\phi_T^E/\phi_T^E$	$\Delta J/J$
Δv_{DS}	-1.53×10^{-4}	-6.80×10^{-5}	-2.59×10^{-3}	1.72×10^{-3}
Δv_{DT}	-4.14×10^{-4}	-1.39×10^{-4}	2.31×10^{-3}	1.71×10^{-3}
ΔC_6	123	33.4	−47.8	19.3

To understand the strong parameter constraints that we obtain with our bound state spectroscopy, it is important to consider the nonlinear dependence of the binding energy on magnetic field. The magnetic field dependence of ϵ_{bind} as it approaches the collision threshold depends sensitively on the exact shape of the long range interatomic potentials, which are mainly characterized by the van der Waals coefficient, C_6. At magnetic fields far from resonance, the bound state wave function is confined to short internuclear distance and the binding energy varies linearly with magnetic field. The linear dependence on B-field gives relatively little information about C_6. As the B-field approaches resonance, the detuning decreases until the bound state lies just below threshold. Now the bound state wave function penetrates much deeper into the classically forbidden region, which causes ϵ_{bind} to curve toward threshold as a function of magnetic field. Because the energetically forbidden region stretches out as C_6/r^6, the observed curvature depends sensitively on the C_6 coefficient. One can show [26] that an analytical Feshbach model that includes the correct potential range and background scattering processes [27] can reproduce the binding energy curve over the full range of magnetic field.

The coupled-channels theory used in this work applies to two-body scattering; therefore, this theory cannot account for many-body effects in the atom-molecule BEC system, such as a mean-field shift to the observed oscillation frequency [17, 28]. Any such mean-field shift must be fractionally largest near the Feshbach resonance, where the binding energy approaches zero while the atom-atom scattering length increases to infinity. We searched for a mean-field shift to the oscillation frequency when $\mathrm{B}_{\mathrm{evolve}}$ was decreased to ∼156 G. As shown in Fig. 2, the lowest magnetic field data display a clear frequency shift with respect to the coupled-channels theory prediction. As $\mathrm{B}_{\mathrm{evolve}}$ approaches resonance, the observed shift increases to 1.7 kHz, which significantly exceeds a simple estimate for the average atom-atom mean-field shift in the BEC: $4\pi\hbar^2\langle n\rangle a/m \simeq 0.5$ kHz at $\mathrm{B}_{\mathrm{evolve}}$=156.1 G. We are presently investigating new experimental techniques to further study the mean-field shifts, including their density dependence.

Since the lowest frequency data show evidence for a mean-field shift, we exclude these points from the (two-body) theory fit. We determine the cutoff magnetic field for the excluded region by the following procedure. We fit the data set that includes all frequency measurements satisfying $\nu_0 \geq 9$ kHz. Eliminating the lowest frequency point from the set causes the reduced χ^2 to decrease from 0.3 to 0.2, and there is no significant change in parameter values. In contrast, adding the next lower frequency point increases the reduced χ^2 to 1.9, causing a systematic shift in the parameter values. The observed behavior seems sensible since we expect mean-field shifts to increase rapidly as one moves toward resonance (see Fig. 2).

As a result of the improved determination of the ^{85}Rb Feshbach resonance parameters, we find that our new value for the off-resonant or background scattering length, a_{bg}=-443(3) a_0, is inconsistent with the value given in Ref. [14], where a_{bg}=-380(21) a_0. The most plausible explanation we can find for disagreement is that the theoretical expression used to relate measured rethermalization rate to cross section is insufficient for the requisite level of accuracy. However, the new value for a_{bg} allows us to revise our previous estimate for the stability condition of a BEC with negative scattering length [22]. We use Eq. (1) to obtain the linear slope of scattering length versus B-field near B=$\mathrm{B}_{\mathrm{zero}}$. We then find the stability coefficient for BEC collapse, k_{collapse}, by combining the value of $\Delta a/\Delta B$=-39.87(22) a_0/G with the measured slope of 1/$\mathrm{N}_{\mathrm{crit}}$ versus magnetic field [22] of 0.00126(3) (atoms G)$^{-1}$. Thus, we obtain the revised value k_{collapse}=0.547(58), where the error is dominated by a 10% systematic uncertainty in the determination of $\mathrm{N}_{\mathrm{crit}}$. The present determination agrees with the theoretical value of 0.55 [29].

In conclusion, we present a unique method for exploring a ^{85}Rb Feshbach resonance. The observed atom-molecule coherence allows us to study the highly nonlinear dependence of the molecular binding energy on magnetic field. We find good agreement with an analysis of van Kempen et al. [15] and improved precision for the characterization of the Feshbach resonance. In addition, we observe mean-field shifts to the binding energy, offering the possibility for future studies of many-body effects in this exciting system.

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[1] H. Feshbach, Ann. Phys. **5**, 357 (1958), H. Feshbach, *ibid.* **19**, 287 (1962), H. Feshbach, *Theoretical Nuclear Physics* (Wiley, New York, 1992).

[2] E. Tiesinga *et al.*, Phys. Rev. A **46**, R1167 (1992).

[3] P. Courteille *et al.*, Phys. Rev. Lett. **81**, 69 (1998).

[4] J. L. Roberts *et al.*, Phys. Rev. Lett. **81**, 5109 (1998).

[5] V. Vuletić *et al.*, Phys Rev. Lett. **82**, 1406 (1999).

[6] T. Loftus *et al.*, Phys. Rev. Lett. **88**, 173201 (2002).

[7] S. Inouye *et al.*, Nature, **392**, 151 (1998).

[8] S. L. Cornish *et al.*, Phys. Rev. Lett. **85**, 1795 (2000).

[9] E. A. Donley *et al.*, Nature **412**, 295 (2001).

[10] L. Khaykovich *et al.*, Science **296**, 1290 (2002).

[11] K. E. Strecker *et al.*, Nature **417**, 150 (2002).

[12] F. A. van Abeelen and B. J. Verhaar, Phys. Rev. A **59**, 578 (1999).

[13] P. J. Leo, C. J. Williams, and P. S. Julienne, Phys. Rev. Lett. **85**, 2721 (2000).

[14] J. L. Roberts *et al.*, Phys. Rev. A **64**, 024702-1 (2001).

[15] E. G. M. van Kempen *et al.*, Phys. Rev. Lett. **88**, 093201 (2002).

[16] E. A. Donley *et al.*, Nature **417**, 529 (2002).

[17] S. J. J. M. F. Kokkelmans and M. J. Holland, Phys. Rev. Lett. **89**, 180401 (2002).

[18] T. Köhler, T. Gasenzer, and K. Burnett, cond-mat/0209100 (2002).

[19] M. Mackie *et al.*, physics/0210131 (2002).

[20] N. R. Claussen *et al.*, Phys. Rev. Lett. **89**, 010401 (2002).

[21] C. Chin *et al.*, Phys. Rev. Lett. **85**, 2717 (2000).

[22] J. L. Roberts *et al.*, Phys. Rev. Lett. **86**, 4211 (2001).

[23] A. Marte *et al.*, cond-mat/0210651 (2002).

[24] For the ϕ_T^E value, which is not listed in Ref. [23], we used $\phi_T^E = 0.159(18)$ K^{-1} (E. G. M. van Kempen and B. J. Verhaar, private communication).

[25] The value for a_{bg}=-450(3) a_0 was extracted from the Ref. [15] analysis. We refer to this value (as we did also

in Ref. [16]) instead of our earlier experimentally determined value of a_{bg}=-380(21) a_0 [14], which is less precise and less accurate.

[26] S. J. J. M. F. Kokkelmans *et al.*, to be published.

[27] S. J. J. M. F. Kokkelmans *et al.*, Phys. Rev. A **65**, 053617 (2002).

[28] R. A. Duine and H. T. C. Stoof, cond-mat/0210544 (2002).

[29] A. Gammal, T. Frederico, and L. Tomio, Phys. Rev. A **64**, 055602 (2001).