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Photoassociation as a probe of Feshbach resonances in cold-atom scattering

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We investigate theoretically the influence of magnetically tunable Feshbach collision resonances on the photoassociation spectra of ultracold atoms. As an example we consider recently predicted resonances for ^{85}Rb atoms. For excitation to the $^{85}\mathrm{Rb}_2$ $0_g^-(S_{1/2}+P_{1/2})$ electronic state, we predict that the photoassociation rate is resonantly enhanced by at least two orders of magnitude. We find that photoassociation could serve as a useful probe with which to study Feshbach resonances in ultracold collisions. In turn, these resonances should be very important to Bose-condensed gases, and more generally, to coherent atom optics. [S1050-2947(98)50606-3]

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After the first observations of Bose-Einstein condensation (BEC) in dilute, ultracold gases of alkali-metal atoms [1–3], rapid progress has been made in observing and understanding the properties of Bose condensates. Atomic interactions have been found to play a crucial role. Their effect may be accounted for in a mean-field model by a self-energy $4\pi\hbar^2 n(\vec{r})a/m$, where a is the two-body scattering length, m the mass of the atoms, and n their density. In spite of the importance of interactions, in many respects the range of accessible interaction strengths has been rather limited. For example, an important natural scaling parameter for the interaction strength is $\eta = 1.57(N^{1/6}a/a_{HO})^{2/5}$, where a_{HO} is the spread of the zero-point wave function of the trapped atoms and N is their number [4]. For positive scattering length gases, only a very narrow range for η near the value 0.4 has been realized. A negative scattering length gas has also been explored [3], but again under rather limited circumstances. The experiment confirms predictions [5] that condensates can form only if the attractive mean-field energy is less than the spacing of the trap levels. For larger interaction energies the condensate presumably collapses [5], but the physics of such a collapse is as yet unclear.

In order to more fully understand the effect of atomic interactions on dilute Bose condensates, it would clearly be desirable to be able to tune the scattering length to an arbitrary value. This would allow for studies of BEC in very strong or weak interaction limits, and it might also be possible to study the dynamics of the collapse of a condensate induced by a sudden switch of the sign of a. A proposal to produce such variations of the scattering length with magnetic-field-induced Feshbach resonances was published some years ago [6]. Feshbach resonances are scattering resonances that arise when the total energy of a pair of colliding atoms matches the energy of a quasibound two-atom state, leading to the resonant formation of this state during the collision. Magnetic tuning of the resonance is possible if the magnetic moments of the free and quasibound states are different, and this allows for the tuning of the scattering length. A concrete example of this was predicted recently for the case of a ^{85}Rb gas sample in the highest level $(|f,m_f\rangle = |2,-2\rangle)$ of the $f=2$ lower hyperfine manifold [7]. According to this prediction, based on a previous analysis of measured bound $^{85}\mathrm{Rb}_2$ levels [8], a can be given an arbitrary positive or negative value by changing the strength of the magnetic field around a certain resonance value for each of three Feshbach resonances. All of these are in the range where the atoms can be trapped in a static magnetic trap.

The potential importance of these scattering resonances is not necessarily restricted to single-species Bose condensation. For instance, they could allow the tuning of the relative interaction strengths between and within species in a multicomponent Bose condensate. Feshbach resonances might play a role in minimizing interactions within the lasing species in an atom laser. Resonant interactions between coherent beams of atoms might be important, and could occur at a nonzero and sharply defined value of the relative kinetic energy.

Experimental studies of these collision resonances are clearly desirable, in order to determine the quantum numbers of the resonances, the field values at which resonances occur as a function of collision energy, and the resonance widths. We propose a method to observe and study Feshbach resonances based on cold-atom photoassociation (PA) [9]. In this process, a photoassociation laser optically excites two colliding ground-state atoms into a bound electronically excited molecular state. We predict a dramatic increase of the PA signal for magnetic-field strengths in the vicinity of a Feshbach resonance; the resonant formation of the quasibound two-atom state increases the penetration of the colliding atoms to the distance range where the optical excitation occurs. This enhancement of the PA signal should serve as a clear-cut signal for the occurrence of a Feshbach resonance at the experimental field strength. To be concrete, we consider the specific example of the predicted Feshbach resonances of ^{85}Rb [7], but many of the conclusions of this analysis should apply more generally.

An alternative method to observe and study Feshbach resonances would be through their impact on the thermalization of an ultracold gas [10], or on the properties of a Bose-condensed gas. However, photoassociation has certain advantages over studies of gas properties that should make this technique of some interest. First, studies of gas properties at many different field values are rather cumbersome and difficult to carry out. In contrast to this, photoassociation provides a very rapid and direct signature of a collision resonance. This could be particularly important when searching for a very narrow resonance. Further, the analysis of gas thermalization experiments becomes very complicated once the elastic collisions are energy dependent and no longer purely s wave. With photoassociation, selecting the 0_g^- electronic state connected to the $S_{1/2}+P_{1/2}$ separated-atom limit as the final state circumvents this problem. This state has total electronic angular-momentum quantum number $j=0$ and, therefore, imposes the selection rule $l=J$ for the partial wave l of the ground-state collision that can give rise to the formation of a given excited two-atom rotational state J [11]. Thus, one can study all partial waves separately. Finally, the laser frequency is an extra parameter available experimentally that allows one to study the energy dependence of the resonance phenomenon through careful analysis of the PA line shapes. In fact, scanning both the laser frequency and the magnetic field makes for an ideal kind of spectroscopy for exploring the structure of the region between the lowest and highest hyperfine-split dissociation limits. One would expect similar resonances in other partial-wave channels at higher temperatures and in other hyperfine entrance channels if the atoms are not polarized.

To illustrate the usefulness of the photoassociation method for the detection and study of field-induced resonances, we calculate the expected PA signal for the broadest of the three predicted ^{85}Rb resonances, which is also predicted to occur at the lowest field strength, i.e., 142 G. We consider a specific temperature (0.3 mK) for the ^{85}Rb gas sample and a linearly polarized PA laser beam propagating in the direction of the magnetic field. For the sake of definiteness we consider the excitation of a specific vibrational level of the lower 0_g^- state with a $J=0$ level energy at $-3.365\ \mathrm{cm}^{-1}$ with respect to the barycenter of the $S_{1/2}+P_{1/2}$ dissociation limit. Due to the $l=J$ selection rule, the Feshbach resonance considered should only show in the PA signal for the excitation of $J=0$ rovibrational levels. Finally, we assume low enough laser intensities that saturation effects can be neglected.

Since the 0_g^- excited state is purely triplet, in the calculation of the PA intensity, only the part $P_{S=1}\psi_c$ of the ground-state collisional wave function ψ_c contributes to the optical matrix element. Here, $P_{S=1}$ is a projection operator on the triplet spin subspace, while ψ_c describes both the relative motion of the atoms and the electronic and nuclear spin dynamics, and is energy normalized. $P_{S=1}\psi_c$ follows from a coupled-channels calculation and is a linear combination of $|S,m_S,I,m_I\rangle$ components:

$$P_{S=1}\psi_c=\sum_{m_S,I,m_I} u_{S=1,m_S,I,m_I}(r;\epsilon)|S=1,m_S,I,m_I\rangle, \quad (1)$$

subject to the requirements of Bose symmetry ($l+S+I=1+I=\text{even}$) and conservation of spin angular momentum about the field direction ($m_S+m_I=-4$). The partial width γ_L for the laser excitation is then given by

$$\gamma_L(\epsilon)=\frac{2\pi I_L}{\varepsilon_0 c}\sum_{I,m_I}\left|\sum_{m_S}\int_0^\infty u_f(r)\langle j,m_j=0,0|[\vec{d}_1+\vec{d}_2].\vec{\sigma}_L|S=1,m_S\rangle u_{S=1,m_S,I.M_I}(r;\epsilon)\ dr\right|^2, \quad (2)$$

with ϵ the collision energy, I_L the laser intensity, $\vec{\sigma}_L$ its polarization vector, $u_f(r)$ the radial wave function of the final state, and $\vec{d}_1$ and $\vec{d}_2$ the atomic electric dipole operators. Compared to Eq. (3) of Ref. [11], a coherent sum over m_S and an incoherent sum over I,m_I have been added. This simple treatment of the nuclear spin is possible because of the selection of the 0_g^- state, which avoids a complicated ‘‘hyperfine spaghetti’’ structure of the PA spectrum. The second-order Zeeman broadening of the 0_g^- state is negligible compared to the width γ_0 due to spontaneous decay, despite the relatively strong magnetic field.

Figure 1 shows the laser frequency dependence of the expected PA signal, in arbitrary units, for a number of B values close to the resonance field value and two nonresonant fields. The abscissa is the laser detuning Δ_L relative to the energy difference between the asymptotic ground hyperfine state and the above-mentioned final vibrational level. We find a dramatic resonance enhancement close to $B=143$ G; the PA maximum grows to a value at least two orders larger than the nonresonant background value. A gradual shift of the maximum to the right, combined with an almost constant width at half maximum, is noticeable for increasing field values. The width of the peaks corresponds approximately to γ_0.

To illustrate the origin of the increased PA maximum, in Figs. 2(a) and 2(b) we show the radial wave functions for the hyperfine components $|f_1,m_{f1},f_2,m_{f2}\rangle$ of ψ_c for $\epsilon=0.3$ mK and two values of B: one close to the resonance value and one further off. The resonant enhancement of the penetration, due to the admixture of the quasibound two-atom state in ψ_c, is clearly visible in the form of a large increase of the spin components that are formed by the promotion of one or both atoms from the lower hyperfine manifold $f=2$ to $f=3$. The shift in the location of the PA maximum is due to the approach of the total energy at resonance to the threshold of the $|f_1,m_{f1},f_2,m_{f2}\rangle=|2,-2,2,-2\rangle$ incident channel, reducing the resonant collisional kinetic energy ϵ_{res} and thus increasing the resonant laser frequency. This is consistent with the predicted pattern of the $a(B)$ dependence [7]: a decrease to $-\infty$, followed by a decrease from $+\infty$ for increasing B, pointing to a quasibound state that crosses the threshold from above (see Fig. 3).

A more detailed investigation of the partial width γ_L for the laser excitation enables a qualitative explanation of all the main features of Fig. 1. In Fig. 4 we show the dependence of γ_L on the collision energy ϵ for a value of B close to the resonance field. A clear resonance behavior is visible superposed on a nonresonant background. The resonant part is described approximately by a Breit-Wigner-like factor $(\Gamma/2\pi)/[(\epsilon-\epsilon_{res})^2+\frac{1}{4}\Gamma^2]$ with $\Gamma(B)$ the resonance width. Figure 4 also shows a Breit-Wigner fit to $\gamma_L(\epsilon)$. The width

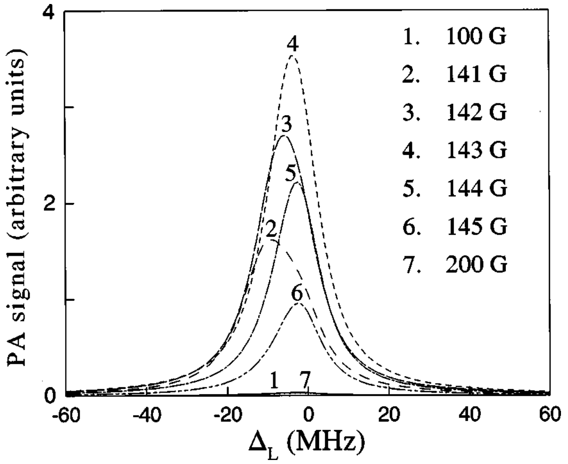

FIG. 1. Calculated photoassociation signal as a function of laser frequency for the ^{85}Rb Feshbach resonance in arbitrary units, for five B values near the resonance field value and two values further off.

turns out to be at most of order 0.2 mK. We find that $\epsilon_{res}(B)$ shows approximately a linear B dependence, as one would expect for a state that crosses the threshold to become bound. It is interesting to note, however, that the crossing ($\epsilon_{res}=0$) appears to occur at a field somewhat larger than where the scattering length becomes infinite ($B=142$ G), due to interference of the resonance with the background for small ϵ_{res}.

Retaining only the Feshbach resonance contribution to γ_L and describing it by the above Breit-Wigner form, the photoassociation rate constant

$$K(T,B,\omega_L)=\left\langle v\frac{\pi}{k^2}\frac{\gamma_0\gamma_L}{[\epsilon+\Delta_L]^2+\frac{1}{4}\gamma_0^2}\right\rangle, \qquad (3)$$

with the brackets $\langle\ \rangle$ standing for a thermal average over the collision velocity v and the associated wave number k, factorizes into the ϵ integral

$$T^{-3/2}\int_0^\infty d\epsilon\ \exp-\epsilon/kT\frac{1}{[\epsilon+\Delta_L]^2+\frac{1}{4}\gamma_0^2}\ \frac{\Gamma/2\pi}{[\epsilon-\epsilon_{res}]^2+\frac{1}{4}\Gamma^2} \qquad (4)$$

and a factor K_0 independent of T, B and ω_L. Γ is sufficiently small compared to the two remaining energy scales kT and γ_0 occurring in the integral (4), for a qualitative

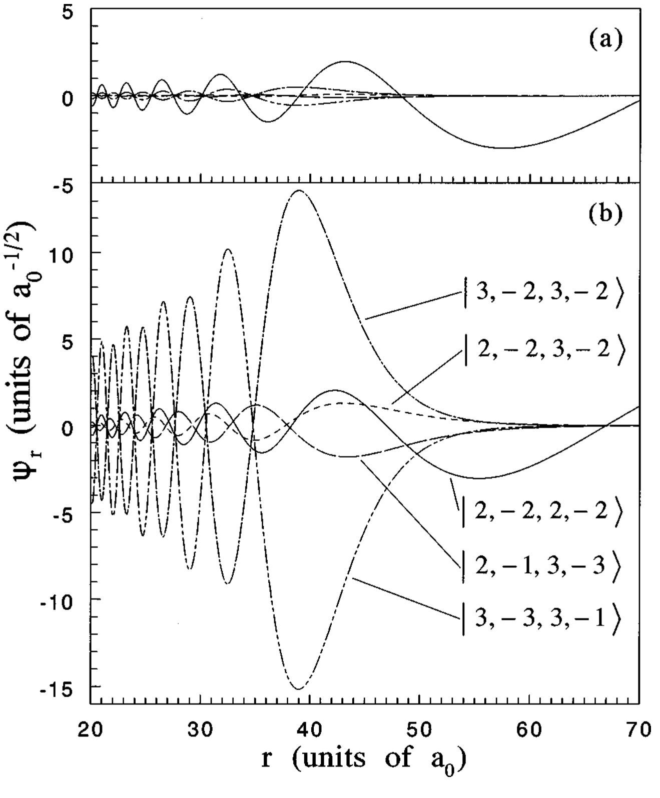

FIG. 2. Radial wave functions $\Psi_r(r)$ for the hyperfine components $|f_1,m_{f1},f_2,m_{f2}\rangle$ of the ground-state collisional wave function. (a) Field far from resonance ($B=100$ G). (b) Field close to resonance ($B=143$ G). Resonant admixture of a quasibound two-atom state enhances the interior wave functions.

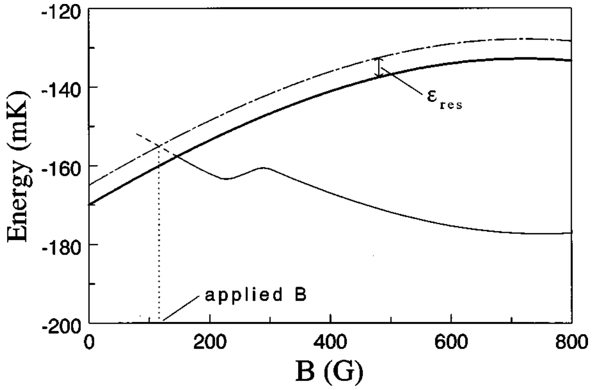

FIG. 3. Bound-state energy (thin solid line) and entrance channel threshold (thick line) as a function of the magnetic-field strength B. The dashed extrapolation of the bound-state curve is a symbolic representation of a quasibound state embedded in the continuum. A Feshbach resonance occurs when the total energy (threshold plus kinetic energy; dashed-dotted line) equals the quasibound-state energy at the applied magnetic field. For clarity the figure shows a situation where the resonant kinetic energy ϵ_{res} is higher than the energies that contribute to the PA signal at experimental temperatures.

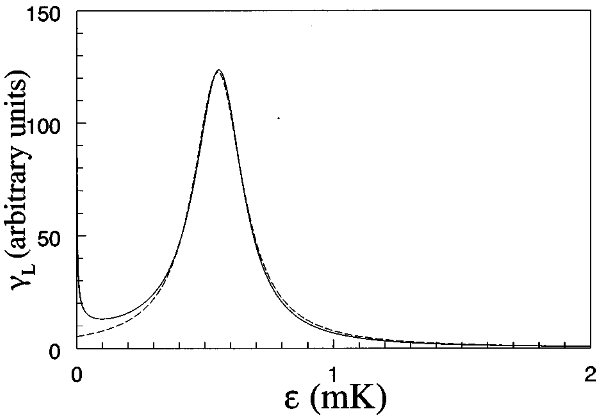

FIG. 4. Dependence of partial width γ_L (solid line) for laser excitation on collision energy ϵ close to resonance and a Breit-Wigner fit to this curve (dashed line).

description in which we approximate the Feshbach resonance energy dependence by a Dirac δ function and obtain

$$K(T,B,\omega_L)=K_0T^{-3/2}\ \exp(-\epsilon_{res}/kT)\frac{1}{[\epsilon_{res}+\Delta_L]^2+\frac{1}{4}\ \gamma_0^2}. \tag{5}$$

Equation (5) describes the qualitative features of the PA signals with 141 $G<B<143$ G displayed in Fig. 1: (1) a shift of the signals from $\Delta_L=0$ over $\epsilon_{res}(B)$ in the negative Δ_L direction; (2) a width approximately equal to the spontaneous emission rate γ_0; (3) a decrease in magnitude of the PA maximum with increasing resonance energy above threshold. The decrease of the signal with increasing B above 143 G can be ascribed to the gradual disappearance of the resonance below threshold.

We conclude that magnetic-field-induced Feshbach resonances will be readily observable in a photoassociation experiment carried out on a ^{85}Rb gas sample. We predict a strong enhancement of the PA signal, with a dependence on the laser frequency and the magnetic field that can be qualitatively understood by considering the limit of a vanishing width of the Feshbach resonance. The laser detuning at the maximum of the PA signal immediately gives the resonant kinetic energy at the experimental field. The observation of the PA spectral peak for varying B could enable the first experimental demonstration of the shift of a Feshbach resonance into the continuum, starting from a bound two-atom state that crosses the threshold of the elastic-scattering channel. An interesting alternative possibility to study this phenomenon could be realized via a two-photon experiment, where two atoms in the $|f_1=3,m_{f1}=-3\rangle+|f_2=3,m_{f2}=-3\rangle$ entrance channel collide in the presence of two laser fields of frequency ω_1 and ω_2 that enable a two-photon transition to the above-mentioned bound state. Again, varying the magnetic field, the latter could be tuned to above threshold.

For these reasons, photoassociation spectroscopy appears well suited as a probe of Feshbach resonant collisions, and more generally as a spectroscopic probe of the structure of the region between the lowest and highest hyperfine-split two-atom dissociation limits. Such scattering resonances should provide new opportunities to study Bose-Einstein condensates with a wider range of interaction strengths, and may have other applications in atom optics. We finally note that very precise measurements of the magnetic-field values at which the collisions are resonant could more precisely determine interatomic potentials.

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