PHYSICAL REVIEW A **81**, 041603(R) (2010)

# Microwave-induced Fano-Feshbach resonances

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(Received 2 October 2009; published 15 April 2010)

We investigate the possibility to control the $s$-wave scattering length for the interaction between cold bosonic atoms by using a microwave field. Our scheme applies to any atomic species with a ground state that is split by hyperfine interaction. We discuss more specifically the case of alkali-metal atoms and calculate the change in the scattering length for $^{7}$Li, $^{23}$Na, $^{41}$K, $^{87}$Rb, and $^{133}$Cs. Our results yield optimistic prospects for experiments with the four latter species.

DOI: 10.1103/PhysRevA.81.041603 PACS number(s): 03.75.Nt, 37.10.Vz

Cold atomic gases constitute model systems to investigate a wealth of collective quantum phenomena, ranging from few-body physics [1,2] to condensed matter problems [3,4]. In particular one can control the strength of the interparticle interactions using scattering resonances that occur in a collision between two atoms with low energy. These so-called Fano-Feshbach resonances (FFR's) arise when the entrance collision channel, with an energy threshold $E_{\mathrm{th}}$, is coupled to another channel that supports a molecular bound state $b$ at an energy $E_{\mathrm{b}}$ close to $E_{\mathrm{th}}$ [1,5–7]. The scattering length that characterizes the $s$-wave scattering between the two atoms has a dispersive variation with $E_{\mathrm{th}} - E_{\mathrm{b}}$, and can, in principle, be tuned to a value with arbitrary sign and magnitude.

In practice, FFR's are generally obtained by adjusting the external magnetic field. One takes advantage of the degenerate structure of the lowest electronic energy level of the atoms. In the case of alkali-metal atoms that are widely used in cold atom experiments, the degeneracy emerges from the spins of the valence electron and of the nucleus. If the magnetic moment of the bound level $b$ is different from that of the entrance channel, the energy difference $E_{\mathrm{th}} - E_{\mathrm{b}}$ can be tuned by scanning the external field. This leads to a resonant variation of the scattering length, with a width that depends on the coupling between the two channels and hence on the details of the interaction between the colliding atoms. For some atomic species, such as Li, K, or Cs, these magnetic FFR's have been an invaluable tool for many studies related to atom-atom interactions [1–4]. However, the absence of external control on the width of magnetic FFR's and their occurrence only for fixed values of the magnetic field may constitute a serious drawback. For Na atoms ($^{23}$Na), for example, the identified resonances are in the 1000 G region with a width around 1 G or less [8,9]. Similar values are found for polarized Rb atoms ($^{87}$Rb) [10]. These large field values and narrow widths severely limit the use of FFR's for these species.

In this Rapid Communication we study an alternative to magnetic FFR's, where the entrance channel is resonantly coupled by a microwave (mw) field to a bound state in another collision channel. All relevant states correspond to the electronic ground level of the atoms, and the resonance is reached by adjusting the frequency of the mw. The width of the resonance is related to the strength of the magnetic dipole coupling between the two channels and is proportional to the mw intensity. Our scheme is reminiscent of optical FFR's, as proposed in [11] and experimentally demonstrated in [12,13]. There, the bound state $b$ was an electronically excited dimer. Although optical FFR's, which rely on electric rather than magnetic dipole coupling, allow, in principle, stronger resonances, their practical use is limited by the unavoidable losses due to spontaneous emission processes. One can also use a pair of laser beams to coherently couple two states from the ground electronic level [14]. However, for a given change of the scattering length this method leads to a similar spontaneous emission rate as in the case of a single-photon excitation [15]. So far the lifetimes of atomic samples submitted to optical FFR were limited to tens of milliseconds, which is likely to be too short to reach a many-body equilibrium state. By contrast mw-FFR's do not suffer from any spontaneous emission process and the associated loss rates should be comparable to those observed with magnetic FFR's.

So far the use of mw or rf fields has been discussed in relation to manipulating existing FFR's [16–18]. Zhang *et al.* [17] proposed considering magnetic FFR's for atomic states dressed by a two-color Raman process or by an rf field. The idea was to provide an independent control of different scattering lengths in multicomponent gases. The rf coupling of several magnetic FFR's has been studied experimentally and theoretically in [18]. The analysis showed that the main role of rf is to couple the bound states that give rise to these resonances. Our idea of inducing new FFR's by using mw fields brings in a novel physical context. We focus on the case of zero static magnetic field, which is presently put forward in the studies of ground-state properties and quantum phase transitions in spinor Bose gases. Such experiments require extremely low magnetic fields (<10 mG), and the manipulation of the interatomic interactions becomes crucial for the observation of quantum transitions and their dynamics. Our scheme is also different from [16] where a resonant oscillating magnetic field was used to enhance the production of diatomic molecules near an existing FFR. In our case the bound state that is coupled to the entrance channel is only virtually populated, and no molecule is produced in the collision.

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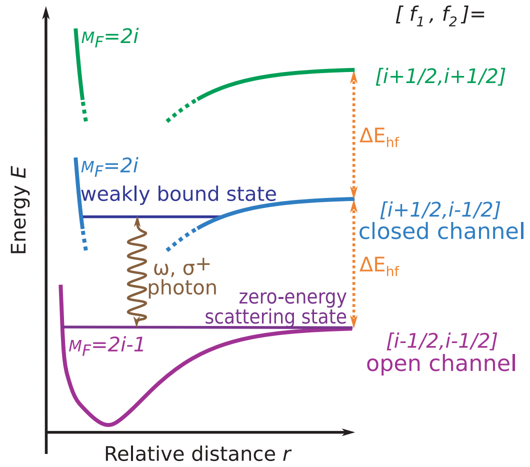

FIG. 1. (Color online) Fano-Feshbach resonance in a collision between two atoms, induced by an oscillatory magnetic field. If the mw frequency $\omega$ approaches the energy difference between the incident scattering state and a weakly bound dimer state, the pair of atoms undergoes virtual spin-flip transitions which cause a resonant variation of the scattering length with $\omega$.

For simplicity we study in the following a collision between two identical bosonic atoms prepared in the same internal state. Our treatment can be straightforwardly extended to fermionic particles and to mixtures of atoms in different internal states. More specifically, we consider alkali-metal atoms whose ground level is split by the hyperfine interaction into two sublevels with total spins $f_+ = i + 1/2$ and $f_- = i - 1/2$, where $i$ is the nuclear spin. The frequency $\omega$ of the mw field is chosen close to the hyperfine splitting $\Delta E_{\mathrm{hf}}$ between these two sublevels (see Fig. 1). The various collision channels can then be grouped into three categories corresponding to asymptotic states with (i) both atoms in $f_+$, (ii) one atom in $f_+$ and one in $f_-$, and (iii) both atoms in $f_-$. We consider in the following the case of a $f_- f_-$ collision and the mw induces a quasiresonant transition to a bound state in a potential from the $f_+ f_-$ group as shown in Fig. 1.

We describe the system in the center-of-mass frame of the atom pair. Neglecting the weak coupling between the atomic spins, the atom-atom interaction is spatially isotropic. We limit our analysis to $s$-wave collisions governed by the radial Hamiltonian (see [19] and references therein)

$$H = \frac{p^2}{2\mu} + V_{\mathrm{c}}(r) + V_{\mathrm{hf}} + \hbar\omega\, a^\dagger a + W = H_0 + W, \quad (1)$$

where $r$ is the interatomic distance, $p$ is its conjugate momentum, and $\mu = m/2$ is the reduced mass of the atom pair. The central part $V_{\mathrm{c}}(r)$ of the interaction is given by $V_{\mathrm{c}}(r) = V_S(r)P_S + V_T(r)P_T$, where $P_S$ and $P_T$ are the projection operators onto the electronic-singlet and triplet subspaces. The term $V_{\mathrm{hf}} = a_{\mathrm{hf}}(\boldsymbol{s}_1\boldsymbol{i}_1 + \boldsymbol{s}_2\boldsymbol{i}_2)$ is the hyperfine interaction, where $\boldsymbol{s}_j$ and $\boldsymbol{i}_j$ stand for the spin operators of the electron and nucleus of atom $j$. We use a quantum description for the mw field and $a^\dagger$ is the creation operator for an mw photon in the relevant mode. The magnetic dipole interaction between the atoms and the mw is $W = -\boldsymbol{M}\boldsymbol{B}$, where $\boldsymbol{M}$ is the total magnetic dipole operator of the atom pair and $\boldsymbol{B} = b_0(\boldsymbol{\varepsilon} a + \boldsymbol{\varepsilon}^* a^\dagger)/\sqrt{2}$ is the magnetic field operator for the mode of polarization $\boldsymbol{\varepsilon}$. As usual in the dressed-atom approach [20], the amplitude $b_0$ and the number of photons $N$ in the mw mode are arbitrary. The only relevant physical quantity is the amplitude of the applied mw field $B_0 = b_0\sqrt{N}$ (with $N \gg 1$). We assume that the magnetic field is $\sigma^+$ polarized with respect to the quantization axis $\boldsymbol{e}_z$.[1] The valence electron in each atom has zero angular momentum and $W$ reduces to[2]

$$W = W_1\,(S^+ a + S^- a^\dagger), \quad (2)$$

where $W_1 = \mu_{\mathrm{B}} b_0/\hbar$, $\mu_{\mathrm{B}}$ is the Bohr magneton and $S^\pm = S_x \pm i S_y$, with $\boldsymbol{S} = \boldsymbol{s}_1 + \boldsymbol{s}_2$ being the total electron spin.

We study the scattering properties of $H$ using two different methods: (i) if the mw Rabi frequency $\mu_{\mathrm{B}} B_0$ is much smaller than the binding energy $|E_T|$ of the dimer and the level spacing in the closed channel, the scattering is well described by a single-resonance two-channel model; (ii) for $\mu_{\mathrm{B}} B_0 \gtrsim |E_T|$, a more general description is obtained through a full coupled-channel calculation.

We first describe method (i). We consider $H$ as a two-channel model [1] where $H_0$ is the bare Hamiltonian and $W$ is the coupling operator. The symmetries of $H_0$ allow the choice of bare open- and closed-channel wave functions which have well-defined photon numbers $N$, total spin $F$, and total spin projection $M_F$ along the quantization axis ($\boldsymbol{F} = \boldsymbol{s}_1 + \boldsymbol{i}_1 + \boldsymbol{s}_2 + \boldsymbol{i}_2$), whereas $W$ directly couples subspaces with $\Delta M_F = -\Delta N = \pm 1$. The coupling term $W$ does not vanish in the limit of infinitely separated atoms. Hence, there is a difference $\Delta$ in the scattering threshold energy of $H$ compared to that of $H_0$. If the detuning $\delta$ of the mw with respect to the single-atom hyperfine splitting $\Delta E_{\mathrm{hf}}$ is greater than $\mu_{\mathrm{B}} B_0$, then $\Delta \sim (\mu_{\mathrm{B}} B_0)^2/\delta$. Method (i) is applicable when $\Delta \ll |E_T|$ and can be neglected. Near resonance, where $|\delta| \sim |E_T|$, this condition requires $\mu_{\mathrm{B}} B_0 \ll |E_T|$.

We start by stating a selection rule associated with $W$. All internal states in the $M_F = 2i + 1$ and $M_F = 2i$ subspaces are electronic-triplet states. More precisely, the $M_F = 2i + 1$ subspace has dimension one, with $|S = 1, I = 2i, F = 2i + 1, M_F = 2i + 1\rangle$ as a basis vector ($I$ determines the modulus of the total nuclear spin $\boldsymbol{I} = \boldsymbol{i}_1 + \boldsymbol{i}_2$). The $M_F = 2i$ subspace has dimension two,[3] and it is spanned by $|\eta_1\rangle = |S = 1, I = 2i, F = 2i, M_F = 2i\rangle$ and $|\eta_2\rangle = |S = 1, I = 2i, F = 2i + 1, M_F = 2i\rangle$. The spatial components of the eigenfunctions of $H_0$ in these subspaces decouple from the internal states and are all eigenfunctions of the triplet Hamiltonian $H_T = p^2/2\mu + V_T(r)$. The bare open- and closed-channel spatial wave functions are thus orthogonal. The operator $W$ does not act on the spatial parts of the wave functions. Hence, its matrix element between an open-channel state with $M_F = 2i$ and a bound state with $M_F = 2i + 1$ is

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[1] This restriction leads to simpler algebra, but is not essential: any polarization can be decomposed into $\sigma_\pm$ components and, for a given $\omega$, only one of the components will induce the desired resonant coupling to a bound state.

[2] In Eq. (2) we omit a small coupling of the mw to the nuclear spins which does not affect the results.

[3] For $s$-wave collisions between bosons, only symmetric internal states are relevant.

zero. Therefore, $W$ cannot induce any resonance between these two subspaces.

We now consider a resonance between the $M_F = 2i - 1$ subspace (dimension five) and the $M_F = 2i$ subspace. For the bare open-channel wave function we choose the $M_F = 2i - 1$ threshold-energy scattering state $|\Psi_{\boldsymbol{k}=\boldsymbol{0}}^{(2i-1)}\rangle$, in the presence of $N$ photons. For large interatomic separations, this state corresponds to the two-particle state $|f_- f_-, F = 2i - 1, M_F = 2i - 1\rangle$ in which both atoms have $f = m_f = i - 1/2$ (see Fig. 1). The bare closed-channel wave function is chosen in the form $|\Psi_0^{(2i)}\rangle = |\varphi_T, \eta_1\rangle$, where $\varphi_T(r)$ is a bound state of $H_T$ and $|\eta_1\rangle$ is defined previously (see Fig. 1).

The single-resonance two-channel model leads to the usual behavior for the scattering length as a function of the frequency $\omega$ close to an FFR resonance

$$a(\omega) = a_{\rm bg}\left(1 + \frac{\Delta\omega}{\omega - \omega_{\rm res}}\right). \qquad (3)$$

The background scattering length $a_{\rm bg}$ corresponds to a collision in the absence of mw, between two atoms in the state $|f = i - 1/2, m_f = i - 1/2\rangle$. The resonance position is given by $\hbar\omega_{\rm res} \approx \Delta E_{\rm hf} - |E_T| + \alpha B_0^2$, where $\alpha B_0^2$ is a small shift due to the coupling between the open and closed channels [1]. The width $\Delta\omega$ of the mw FFR is

$$\hbar\Delta\omega = \frac{1}{2\pi}\,\frac{\mu}{a_{\rm bg}\hbar^2}\,(\mu_{\rm B}B_0)^2\,\left|\left\langle\Psi_0^{(2i)}\middle|S^+\middle|\Psi_{\boldsymbol{k}=\boldsymbol{0}}^{(2i-1)}\right\rangle\right|^2. \qquad (4)$$

It is proportional to the mw intensity $B_0^2$ and to the spin-flip Franck-Condon factor $|\langle\Psi_0^{(2i)}|S^+|\Psi_{\boldsymbol{k}=\boldsymbol{0}}^{(2i-1)}\rangle|^2$.

For a given atomic species, method (i) requires the calculation of $\Psi_{\boldsymbol{k}=\boldsymbol{0}}^{(2i-1)}(r)$ and $\varphi_T(r)$. We account for the spin-recoupling phenomenon [1] through the coupled-channel method [21], encode the short-range physics in the accumulated-phase boundary condition [19,22], and use the relaxation method [23] to solve the resulting two-point boundary-value differential systems.[4]

We performed calculations for $^7$Li, $^{23}$Na, $^{41}$K, $^{87}$Rb, and $^{133}$Cs. We use the hyperfine splittings reported in [24] and the singlet and triplet potentials from [10,25–34]. The accumulated-phase boundary condition is applied at the radii $r_0 = 10\,{\rm a}_0$ for $^7$Li, $r_0 = 16\,{\rm a}_0$ for $^{23}$Na, $^{41}$K and $^{87}$Rb, and $r_0 = 20\,{\rm a}_0$ for $^{133}$Cs. We calculate the initial phases of the zero-energy scattering wave functions at $r_0$ through back-integration using the singlet and triplet scattering lengths [10,27–29,32,35]. The energy derivatives of these phases are taken from [19,28] for $^{87}$Rb and $^{23}$Na, and are calculated for the other species using the triplet and singlet potentials. Our results are given in Table I. In practice we find that the broadest resonance widths $\Delta\omega$, as given by Eq. (4) are obtained by choosing $\varphi_T(r)$ as the highest bound state of the triplet potential. For all considered atomic species except $^{133}$Cs, this is the resonance we report in Table I. However, in the case of $^{133}$Cs, the highest-energy bound state is so weakly bound ($|E_T| = h5\,$kHz) that the hyperbolic behavior of $a$ [Eq. (3)] is not valid for $B_0 \gtrsim 1\,$mG, and we therefore report the resonance obtained with the second-highest bound state of $V_T$ ($|E_T| = h110\,$MHz).

TABLE I. Characteristics of the mw-FFR in $^7$Li, $^{23}$Na, $^{41}$K, $^{87}$Rb, and $^{133}$Cs involving the triplet bound states with energies $E_T$. The width $\Delta\omega$ scales as $B_0^2$ and is given for $B_0 = 1\,$G.

| | $^7$Li | $^{23}$Na | $^{41}$K | $^{87}$Rb | $^{133}$Cs |
|---|---|---|---|---|---|
| $\boldsymbol{\lvert E_T\rvert/h}$ (MHz) | 12,000 | 200 | 140 | 25 | 110 |
| $\boldsymbol{\omega_{\rm res}/2\pi}$ (GHz) | 12 | 1.6 | 0.12 | 6.8 | 9.1 |
| $\boldsymbol{\alpha}$ (kHz/G$^2$) | 0.33 | 6.8 | 21 | 120 | 30 |
| $\boldsymbol{\Delta\omega/2\pi}$ (Hz) | 6 | 1400 | 350 | 60 | −4500 |

The largest resonance width is obtained for $^{133}$Cs ($-4500\,$Hz for $B_0 = 1\,$G). Relatively large widths are also obtained for $^{23}$Na and $^{41}$K. In the case of $^{87}$Rb, the singlet and triplet scattering lengths differ by less than 10% [10]. Hence, the near-threshold properties of the singlet and triplet Hamiltonians are similar. The open- and closed-channel wave functions are thus nearly orthogonal, which leads to a reduction of their overlap and to a narrower resonance. For $^7$Li the triplet scattering length is negative [35] and $H_T$ does not support weakly bound molecular states [1]. The last bound state has a small spatial extent, which leads to an even narrower resonance.

We now turn to method (ii), where we take into account that colliding atoms are asymptotically in dressed atomic states. This method can be used for larger Rabi frequencies, such that $\mu_{\rm B}B_0 \gtrsim \Delta$. We restrict the full Hamiltonian $H$ to the eight-dimensional subspace spanned by all internal states in the $M_F = 2i + 1$, $2i$, and $2i - 1$ subspaces. For given values of $B_0$ and $\omega$, we calculate the eight-component scattering state $|\Psi_{B_0,\omega}\rangle$ of $H$ corresponding, for large interatomic separations, to dressed-state atoms with zero kinetic energy. The scattering length $a(B_0, \omega)$ is extracted from the asymptotic behavior of this wave function. For a given $\mu_{\rm B}B_0 \ll |E_T|$, we checked that we recover the hyperbolic behavior of Eq. (3). We also evaluated the coefficient $\alpha$ giving the shift of the resonance position $\omega_{\rm res}$ (see Table I).

Method (ii) allows us to investigate the mw-FFR in $^{133}$Cs involving the highest bound state of $V_T$, where Eq. (3) is not applicable for $B_0 \gtrsim 1\,$mG. To avoid inelastic processes we assume that the atoms are asymptotically in the lowest atomic dressed state. For large $\delta < 0$, this state corresponds to the two-particle state $|f_- f_-, F = 2i - 1, M_F = 2i - 1\rangle$, and therefore $a = a_{\rm bg} = -2500\,{\rm a}_0$. For large $\delta > 0$ it corresponds to $|f_+ f_+, F = 2i + 1, M_F = 2i + 1\rangle$, with $a = a_T = 2400\,{\rm a}_0$. For $B_0 \lesssim 1$ mG the resonance is hyperbolic, as predicted by method (i) [see Eq. (3)]. For larger $B_0$ the scattering length becomes very large for $\hbar\omega \approx \Delta E_{\rm hf}$, but $a(\omega)$ no longer satisfies Eq. (3). Figure 2 shows how the dependence $a(\omega)$ evolves when $B_0$ increases from 0.1 mG to 1 G. In the $\delta > 0$ region, collisions between atoms in the "stretched" state $f_+ = m_f = i + 1/2 = 4$ occur with a large inelastic rate because of dipole-dipole interactions [36]. Therefore, one should operate in the $\delta < 0$ region, where the contamination of the collision state by the stretched state is small. A detailed modeling of the large-$B_0$ FFR's will be presented elsewhere.

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[4] The same approaches were used for method (ii).

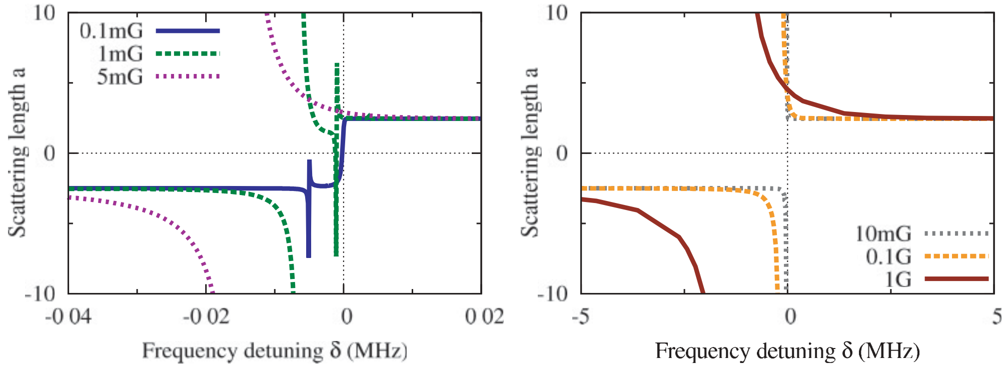

FIG. 2. (Color online) Resonance in $^{133}$Cs involving the bound state with energy $|E_T| = h5\,\mathrm{kHz} = \mu_B 4$ mG, for $B_0$ ranging from 0.1 mG to 1 G, calculated using method (ii). The scattering length $a$ is expressed in units of $1000\,a_0$.

Our results draw optimistic prospects for modifying the scattering length in atomic gases using a mw field. Using small resonant transmitting loop antennas in the near-field regime, it is possible to reach mw magnetic field amplitudes $B_0 \sim 10$ G in the desired frequency range, while keeping a reasonable incident electromagnetic power (below 10 W). The resonance widths obtained for the hyperbolic resonances in all atomic species except $^7$Li are then well above 1 mG, and thus notably exceed typical magnetic field fluctuations in setups with an efficient magnetic shielding. The nonhyperbolic resonance obtained with $^{133}$Cs has a width of the order of 1 G for $B_0 = 1$ G. Our scheme can be readily transposed to fermionic atoms, multicomponent gases, and heteronuclear mixtures, and it can allow for a fine tuning of interspecies interactions in all three cases.

We thank M. Köhl, S. Kokkelmans, F. Gerbier, and Z. Hadzibabic for helpful discussions. We are grateful to S. Kokkelmans for providing us with the singlet and triplet electronic potential curves for Rubidium. This work is supported by Région Ile de France IFRAF, by ANR (Grant No. ANR-08-BLAN-65 BOFL), by the EU project SCALA, and by the Dutch Foundation FOM. LPTMS is a mixed research unit No. 8626 of CNRS and Université Paris Sud. LKB is a mixed research unit No. 8552 of CNRS, ENS, and Université Pierre et Marie Curie.

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