Feshbach resonances in ^{23}Na–^{87}Rb

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Abstract. We describe s-wave collisions between ultracold ^{23}Na and ^{87}Rb atoms in the presence of a magnetic field. For any collision input channel knowledge of the singlet and triplet intermolecular potentials [1] enables us to predict the variation in scattering lengths as a function of the magnetic field. We employ the Born-Oppenheimer approximation to predict several Feshbach resonances for ^{23}Na^{87}Rb. We also include a discussion of why these resonances are expected to be narrow as observed in the case of ^{87}Rb$_2$.

PACS. 34.90.+q Other topics in atomic collisions – 03.75.Hh Multicomponent condensates

1 Introduction

The most important parameter in the description of an ultracold atomic gas is the s-wave scattering length a. At ultracold ($\sim$ microkelvin) temperatures where two-body processes dominate the interactions in the gas, elastic as well as inelastic collisions depend on the singlet (a_S) and triplet (a_T) s-wave scattering lengths [2]. In the case of a Bose-Einstein Condensate (BEC) a determines the rate of evaporative cooling, stability and the mean-field energy of the gas [3,4]. The elastic scattering processes responsible for fascinating phenomena like superfluidity and the existence of phonon-like excitations [5] ultimately depend on a.

In a two-species BEC (TBEC) the interspecies scattering length a_{12} determines the efficiency of sympathetic cooling, the strength of the coupling between the two species [6] and the miscibility of the two components [7]. Importantly, a_{12} can be tuned using a magnetic field [8]. A Feshbach resonance is typically encountered while changing the magnetic field as shown in Figure 1. The resonance occurs when a bound state in the upper molecular well correlating to a closed channel becomes degenerate with the collision energy along the asymptotically open collision channel. For cold atoms the asymptotic energy is set by the dissociation limit of the lower molecular well. At the resonance, the scattering length a_{12} diverges. Feshbach resonances are therefore a unique experimental handle for tuning the interactions in a degenerate gas. They have been used to reach degeneracy for species difficult to condense in zero field [9], to control the explosion and implosion of a BEC [10], and to coherently couple an atomic BEC with molecules [11]. Feshbach

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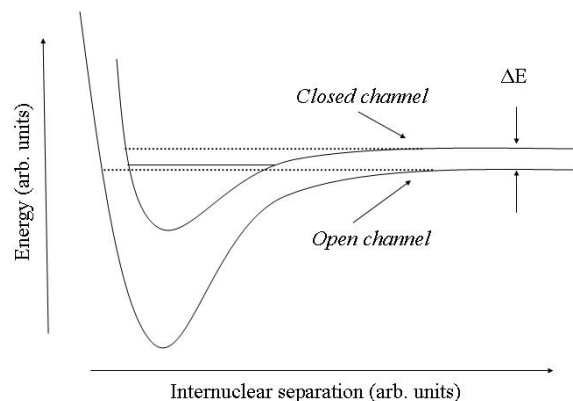
Fig. 1. Bound and scattering states near a Feshbach resonance. The bound state belonging to the upper molecular potential is almost degenerate with the collision energy of the input channel, which is a little higher than the dissociation energy of the lower molecular potential. The separation between the channels is provided by the energy ΔE, arising from hyperfine and Zeeman interactions.

resonances have also been employed to create bright solitons [12], ultracold molecules [13], a strongly interacting Fermi gas [14], and a molecular BEC [15]. A superfluid phase transition [16] has been probed using a Feshbach resonance. Closer to the treatment in this paper is the use of Feshbach spectroscopy for the precise determination of interatomic interaction parameters and molecular structure near dissociation: Greiner et al. [14] have created perhaps the most weakly bound diatomic molecular state ever observed, with a binding energy of $\sim 10^{-9}$ cm^{-1}.

Experimentally, Feshbach resonances are typically detected and characterized using variables such as the rates

of rethermalization [17], photoassociation [18], and inelastic loss [19], as well as variations of the mean-field expansion energy of a BEC [20].

While Feshbach resonances have been quite thoroughly explored in homonuclear collisions [19], the study of heteronuclear systems is only just beginning. To our knowledge theoretical calculations exist only for KRb [21] and LiH [22] and for ^{85}Rb^{87}Rb [23]. On the experimental side the first reports of heteronuclear Feshbach resonances (in Na–Li [24] and K–Rb [25]) have only recently appeared. These developments are interesting because in general the Feshbach spectrum in heteronuclear species is richer than in the homonuclears, as pointed out in Section 2.2 below. Two species Feshbach resonances are the first step in the study of ultracold Bose-Fermi mixtures with tunable interactions. Predicted phenomena in these systems include boson-mediated Cooper pairing [26,27], phase separation [28] and supersolid order [29].

The layout of the paper is as follows. In Section 2 we describe the channels available to the collision in the presence of a magnetic field. In Section 3 we account for the mixing of these channels by the molecular exchange potential. In Section 4 we phrase a semi-classical solution to the full coupled-channel problem in terms of the Born-Oppenheimer approximation. In Section 5 we present values of some Feshbach resonances in the ^{23}Na–^{87}Rb system.

2 Channels for the s-wave collision

We describe the entrance channels to the s-wave collision, including the labelling of the atoms and atom-pairs, and choose a particular collision threshold to display the effective Hilbert space in which the collision occurs.

2.1 One-atom states

We consider ^{23}Na and ^{87}Rb atoms in the ground state in the presence of a magnetic field, B. The Zeeman shifts due to B may be comparable or larger than the atomic hyperfine splitting energies (Fig. 2). Due to the non-zero value of B the atomic angular momentum f is not conserved, only m_f, its projection along the direction of the magnetic field, is. Nonetheless the atomic states can be labelled in an $|f, m_f\rangle$ basis since the energy eigenvalues shown in Figure 2 only intersect at rather high values of B (167 kG for ^{23}Na [30], for example). The intersections occur when the magnetic dipole moment of the nucleus (which has been neglected in the values shown in Fig. 2) is taken into account. This occurs at high values of B since the nuclear gyromagnetic ratio is much smaller than the electronic one. We will be considering $B \leq 1$ kG which means f can still be used to label the states. Now in the very high field limit when all the spins align themselves along B the appropriate basis is defined by the magnetic substates $m_{s,i}$ of the electronic (s) and nuclear (i) spin: $|s, m_s\rangle|i, m_i\rangle$. The transformation between the two bases
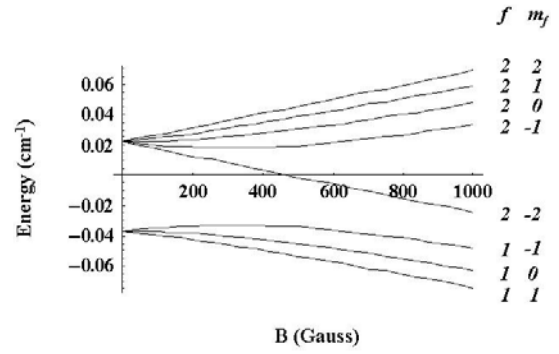
Fig. 2. Hyperfine and Zeeman energies of the $|f, m_f\rangle$ states of ^{23}Na in a magnetic field.
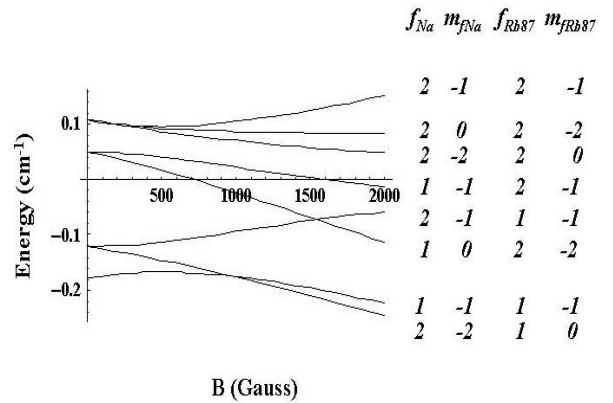
Fig. 3. Hyperfine and Zeeman energies for $|f_{\mathrm{Na}}m_{f\mathrm{Na}}\rangle|f_{\mathrm{Rb}87}m_{f\mathrm{Rb}87}\rangle$ states of ^{23}Na–^{87}Rb atom-pairs with total angular momentum projection $m_{f\mathrm{Na}} + m_{f\mathrm{Rb}87} = -2$ along the magnetic field B. The two threshold crossings shown occur at 994 G and 1551 G respectively.

is magnetic field-dependent:

$$|f, m_f\rangle = C(B)|s, m_s\rangle|i, m_i\rangle \qquad (1)$$

where $C(B)$ is a matrix that reduces to a simple Clebsch-Gordan transformation in the zero-field limit:

$$C(0) = \langle s, m_s, i, m_i|f, m_f\rangle. \qquad (2)$$

2.2 Two-atom states

The two-atom collision channel is written as a direct product of the respective one-atom states, and is an eigenstate of the *collision* basis $|f_{\mathrm{Na}}, m_{f\mathrm{Na}}\rangle|f_{\mathrm{Rb}87}, m_{f\mathrm{Rb}87}\rangle$. The sum of the hyperfine and Zeeman energies for an atom-pair in an eigenstate of the collision basis is the threshold energy of the collision. The variation of the collision thresholds with magnetic field is shown in Figure 3 for the manifold of states with angular momentum projection $m_{f\mathrm{Na}} + m_{f\mathrm{Rb}87} = -2$ along the magnetic field. We note

that the energetically lower crossing between the states $|1,-1\rangle|1,-1\rangle$ and $|2,-2\rangle|1,0\rangle$ occurs at 994 G. The energetically higher crossing between the states $|2,-1\rangle|1,-1\rangle$ and $|1,0\rangle|2,-2\rangle$ occurs at 1551 G.

In contrast to the case of the homonuclears, it is interesting to note the effects of the lack of symmetry in the heteronuclear pair. Since the hyperfine constants are unequal for the two atoms, there are 4 rather than 3 zero-field collision asymptotes. In all, the ^{23}Na^{87}Rb ground state manifold consists of 64 spin states as opposed to 36 for ^{23}Na$_2$ or ^{87}Rb$_2$. This implies that the Feshbach spectrum of heteronuclear diatomics is in general richer than that of the homonuclears.

3 The exchange potential

As atoms approach each other during the collision they experience strong molecular exchange interactions which can be written as

$$V_{Ex} = V_S P_S + V_T P_T \tag{3}$$

where $V_S(V_T)$ are the singlet (triplet) potentials respectively and $P_S(P_T)$ are projection operators on to the singlet (triplet) subspaces. The potentials V_S and V_T for Na–Rb were assembled in [1]. We use the same potentials for our analysis here, and quote the ^{23}Na–^{87}Rb scattering lengths from Table II in the same paper: $a_S = 55^{+3}_{-3}$ Å and $a_T = 51^{+9}_{-6}$ Å.

The $|f_{\text{Na}}, m_{f\text{Na}}\rangle$ $|f_{\text{Rb87}}, m_{f\text{Rb87}}\rangle$ states are mixed by the exchange energy. By considering the commutation relations of the $P_{S,T}$ with the various angular momenta, we find that the exchange potentials couple states which have the same magnetic component of the total angular momentum $(m_{f\text{Na}} + m_{f\text{Rb87}})$ as the input channel for the collision. Interesting dynamical events can happen in this restricted Hilbert space. If, as a result of the collision, either or both atoms in the input channel exit on a different channel, a *spin exchange* collision can occur [30]. If the spin-reorientation energy is larger than the depth of the external potential confining the cold atoms, spin-exchange may result in loss of atoms from the trap. Loss will also happen if the trap is magnetic and the final spin state is not magnetically trappable.

The appropriate basis in the regime of strong molecular interactions is $|S, M_S\rangle|I, M_I\rangle$, where $S(I)$ is the electronic (nuclear) spin and $M_{S(I)}$ its projection along the magnetic field. The recoupling from the collision basis to the molecular basis is magnetic-field dependent:

$$|f_{\text{Na}}, m_{f\text{Na}}\rangle|f_{\text{Rb87}}, m_{f\text{Rb87}}\rangle = R(B)|S, M_S, I, M_I\rangle \tag{4}$$

where $R(B)$ can be expressed in terms of Clebsch-Gordan coefficients and a Wigner 9J symbol in the zero-field limit:

$$
\begin{aligned}
R(0) = \sum_{FM_F} & \langle SM_S IM_I | FM_F \rangle \\
& \times \langle FM_F | f_{\text{Na}} m_{f\text{Na}} f_{\text{Rb87}} m_{f\text{Rb87}} \rangle \\
& \times \sqrt{(2f_{\text{Na}}+1)(2f_{\text{Rb87}}+1)(2S+1)(2I+1)} \\
& \times \begin{Bmatrix} s_{\text{Na}} & i_{\text{Na}} & f_{\text{Na}} \\ s_{\text{Rb87}} & i_{\text{Rb87}} & f_{\text{Rb87}} \\ S & I & F \end{Bmatrix}
\end{aligned}
\tag{5}
$$

where F and M_F are the total angular momentum of the atom-pair and its projection along the magnetic field. Equation (4) implies that the magnetic moments of the atom-pair thresholds and the bound molecular states are unequal. It is precisely this difference that allows resonance-tuning of molecular bound states past atom-pair asymptotes, i.e. Feshbach resonances.

Here we have considered only spin-exchange interactions and neglected magnetic spin-dipole forces between the two alkali valence electrons. Typically spin-exchange loss rates in magnetic traps are $\sim$10 s^{-1} and spin-dipole loss rates are lower by a factor of 10^{-2}–10^{-4} [4]. Although we neglect them here they have been shown to have important effects on p-wave Feshbach resonances and offer a way to tune anisotropic interactions in a cold atomic gas [31]. We note that dipolar relaxation also determines the lifetime of BEC in hydrogen [32] and influences the operation of atomic clocks [33]. We also point out our neglect of relativistic spin-orbit effects which are of the same order but opposite sign as spin-dipole interactions. In Cs losses due to these spin-orbit effects initially prevented the achievement of BEC [4].

4 The Born-Oppenheimer approximation

The full multi-channel collision is described by a set of coupled Schrodinger equations [34] with the Hamiltonian

$$H = K.E. + V_{HFS} + V_B + V_{Ex} \tag{6}$$

(where $K.E.$ is the nuclear kinetic energy) and the wavefunction

$$|\psi\rangle = \phi_1(r)|\chi_1\rangle + \sum_{i \neq 1} \phi_i(r)|\chi_i\rangle \tag{7}$$

where the first state on the right hand side of equation (7) corresponds to the entrance or "open" channel in the collision and the second term to the coupled but "closed" channels. The kets denote the spin and the ϕ_i's the spatial or "orbital part" of the atom-pair wavefunction.

We solve equation (6) for every value of the magnetic field B within the Born-Oppenheimer (BO) approximation. We clamp the nuclei, i.e. neglect the nuclear kinetic energy and diagonalize the full interaction given by

$$V_{int} = V_{HFS} + V_B + V_{Ex} \tag{8}$$

for every value of the internuclear distance R, thus deriving a set of BO potentials. Next we include the nuclear kinetic energy and solve for the bound states of motion along the BO potentials for the diatomic molecule. We repeat this procedure for several values of the magnetic field. The BO potentials for 0, 600 G, and 900 G [35] are shown in Figures 4a, 4b, 4c and 4d where the spin structure becomes progressively more manifest with increasing magnetic field. We also track the (nonlinear) motion of the bound states as a function of the magnetic field as described below.

By diagonalizing the interaction V_{int} we effectively work with single-channel states which are no longer coupled to each other. The justification for doing this comes from two observations. First, none of the resonance values calculated in Section 6 lie within the atomic kinetic energy spread (nK) of either of the two threshold crossings (at 994 and 1551 G) shown in Figure 3. This means the atom-pairs are always prepared in a single eigenstate of the collision basis. Second, for no value of B are there crossings, for any internuclear distance R, among the set of BO potentials. Thus we are justified in making a single-channel approximation in order to describe both the entrance channel for the collision as well as the bound state motion in each of the higher lying wells.

5 Feshbach resonances in ^{23}Na–^{87}Rb

5.1 Resonance values

In order to find the Feshbach resonances for a given channel, we select an open channel and inspect the near-lying bound states of the BO potentials that have a higher dissociation energy than the open channel. Figures 5–7 illustrate some typical resonances for the manifold shown in Figure 3.

In all we found six resonances in this manifold. These have been tabulated in Table 1. The uncertainties in the resonance field values have been calculated from the uncertainty in the potentials.

5.2 Resonance widths

The s-wave collision channels are mixed by the molecular potential described by equation (3), which can be rewritten in the form

$$V_{Ex} = (V_S - V_T)P_S + V_T. \tag{9}$$

From equation (9) we can see that the off-diagonal elements between the collision channels are proportional to $(V_S - V_T)$. These are the interchannel couplings that cause spin-exchange collisions as well as govern the width of the Feshbach resonances. Now, in the Born approximation, the scattering amplitude f is the Fourier transform of the potential V. Therefore $(V_S - V_T)$ is the inverse Fourier transform of $(f_S - f_T)$. For an s-wave collision the scattering amplitude is exactly equal to the scattering length [36].
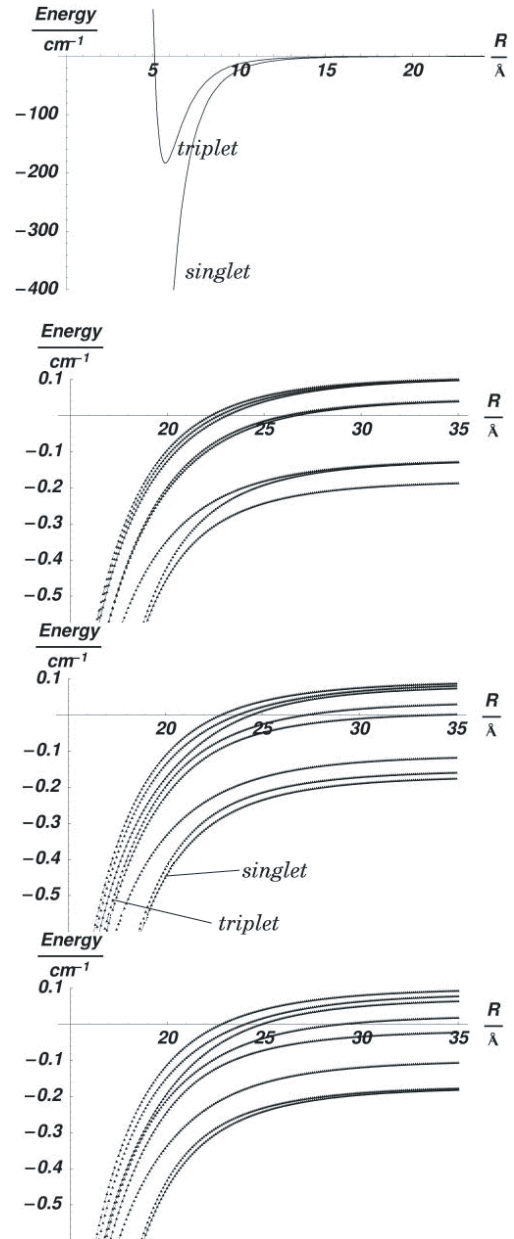

Fig. 4. ^{23}Na^{87}Rb Born-Oppenheimer potentials (see [35]) for the $m_{f\mathrm{Na}} + m_{f\mathrm{Rb87}} = -2$ collision channels for various magnetic fields B. In the uppermost frame ($B = 0$) the hyperfine splitting energies are too small to be evident on the scale of the singlet and triplet energies. In the next lower frame ($B = 0$) the four hyperfine asymptotes and the correlation of the spin states become clear once the potentials are examined on a finer scale. The last two frames ($B = 600$ G and $B = 900$ G) exhibit more clearly the rich spin structure of the heteronuclear pair.

Hence we see that $(V_S - V_T)$ is the inverse Fourier transform of $(a_S - a_T)$. The near-equality of the scattering lengths in ^{23}Na^{87}Rb ($a_S = 55^{+3}_{-3}$ Å and $a_T = 51^{+9}_{-6}$ Å, [1]) is therefore an indication of small interchannel coupling, and hence of the suppression of spin-exchange collisions as well as of the narrowing of Feshbach resonances.
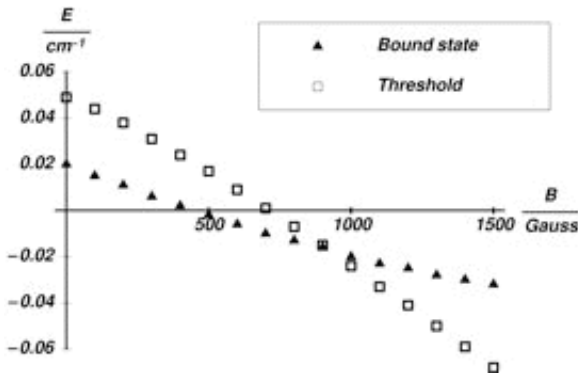
Fig. 5. A Feshbach resonance in ^{23}Na^{87}Rb at 921 G. An atom pair prepared in the open channel $|1\ \ 0\rangle|2-2\rangle$ is resonant with the 21st bound state of the well correlating to the closed collision channel $|2-2\rangle|2\ \ 0\rangle$.
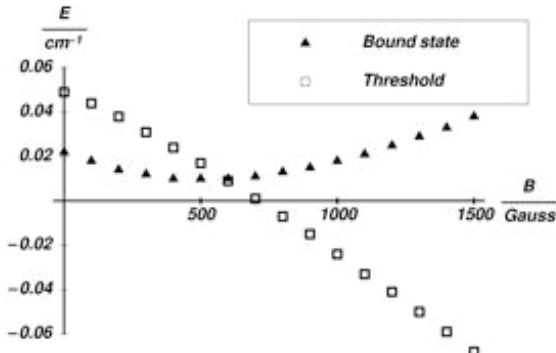
Fig. 6. A Feshbach resonance in ^{23}Na^{87}Rb at 594 G. An atom pair prepared in the open channel $|1\ \ 0\rangle|2-2\rangle$ is resonant with the 21st bound state of the well correlating to the closed collision channel $|2-1\rangle|2-1\rangle$.
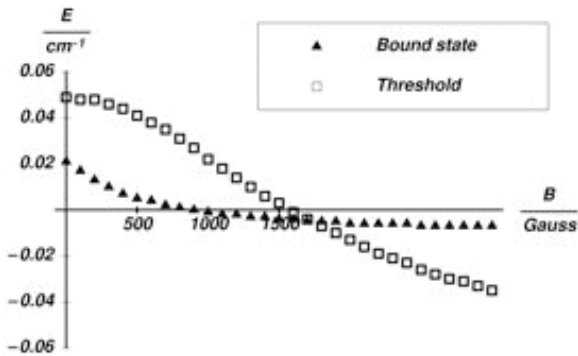
Fig. 7. A Feshbach resonance in ^{23}Na^{87}Rb at 1717 G. An atom pair prepared in the open channel $|1-1\rangle|2-1\rangle$ is resonant with the 22nd bound state of the well correlating to the closed collision channel $|2\ \ 0\rangle|2-2\rangle$.

Physically, the incoming atom-pair flux on a collision channel eventually divides and propagates along the singlet and triplet molecular potentials. The two parts return to where the flux divided with the singlet and triplet components having picked up equal amounts of phase. This constructive quantum interference back into the open channel prevents scattering into other coupled

Table 1. Feshbach resonances in the $m_{f\mathrm{Na}} + m_{f\mathrm{Rb}87} = -2$ manifold in ^{23}Na^{87}Rb. Typical uncertainties in the resonance positions are $\sim \pm 55$ G.

Open channel	$B_{Resonance}$(G)
$|2-1\rangle|2-1\rangle$	1350
$|1\ \ \ 0\rangle|2-2\rangle$	921
$|1\ \ \ 0\rangle|2-2\rangle$	688
$|1\ \ \ 0\rangle|2-2\rangle$	594
$|1-1\rangle|2-1\rangle$	1717
$|1-1\rangle|2-1\rangle$	1061

channels, and hence reduces spin-exchange loss. The suppression of decay mechanisms also enables a large lifetime for the quasi-molecule formed during the Feshbach resonance, and hence a small linewidth for the resonance.

6 Conclusion

The BO approximation is a semiclassical version of the fully quantum mechanical Coupled-Channel (CC) equations. The BO approximation has yielded quite accurate results [34] in the treatment of other species; the difference between the BO and full CC solutions for the resonance positions is usually ~ 1 G. However, a full CC treatment is required for cases where two resonances occurs for the same magnetic field B. In that case quantum interference between the two paths sets in and shifts the positions of the resonances from that predicted by the BO approximation. The CC solutions will also provide the final confirmation of the predicted narrowness of the resonance widths. Efforts are on way to implement the CC solutions, as they are to usefully extend the BO approximation to the isotopomer ^{23}Na^{85}Rb.

In conclusion we have predicted several Feshbach resonances in ^{23}Na^{87}Rb in the Born-Oppenheimer approximation and pointed out the repercussions of the equality of the singlet and triplet scattering lengths on the Feshbach spectrum.

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