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Three Resonant Ultra-Cold Bosons: Off-Resonance Effects

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We solve a finite range two-channel model for three resonant identical bosons. The model provides a minimal description of the various magnetic Feshbach resonances in single species ultra-cold bosonic systems, including off-resonant scattering. We obtain important insights into the interpretation of seminal experiments: the three-body recombination rate measured in Sodium and the Efimov resonances observed in Cæsium. This approach quantifies non universal effects appearing for a finite magnetic field detuning.

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One of the main issues in current ultracold physics is to achieve highly correlated quantum gases. In these studies the magnetic Feshbach resonance is a crucial ingredient: it permits to tune the strength of the two-body interaction measured by the s -wave scattering length to an arbitrarily large value, while the atomic density remains constant. However for dilute bosonic gases, such highly correlated states are very unstable as a consequence of three-body recombinations into deep molecular bound states [1, 2]. Therefore, in the last decade an impressive effort has been made both theoretically and experimentally, for a deep understanding of three-body properties in these systems. Universality concepts borrowed from Nuclear physics together with the specificity of ultracold atoms where an explicit energy scale separation occurs in scattering processes have led to unsuspected physical insights in this domain [3, 4]. For example, the so-called Efimov states have been observed for the first time in a resonant ultracold Cæsium gas [5]. For scattering lengths much larger than the range of inter-atomic forces, Universal Theory [4] permits a powerful analysis of three-body properties without any knowledge of the short range details of the real interatomic forces. For narrow resonances like the one observed in Ref.[2], it is possible to fully determine the Efimov spectrum at resonance using the effective range approach [6, 7]. Despite their success, these approaches are not designed for a description of three-body properties at finite detuning, where off-resonant scattering effects come into play. Experiments on Efimov states in Ref. [9] clearly exhibit some non universal behavior which cannot be taken into account by the Universal Theory. Moreover, the peak in three-body losses in Ref. [2] occurs for relatively large magnetic detuning where the effective range approach is inoperant. In this letter, we solve the three-boson problem by using a two-channel model including the short range character of interatomic forces. The model describes all the various type of magnetic Feshbach resonances: broad, narrow or in the neighborhood of a shape resonance. Results of the model compare quantitatively with experiments of Ref. [2], highlighting the importance

of off-resonant effects in narrow resonances. Concerning the experiments in Refs. [5, 9], our results show that the observed violation of universality follows from the fact that the resonance in the atom-dimer scattering appears in a domain where the range of interatomic forces is not negligible as compared to the scattering length.

We first introduce the finite range two-channel model. The two channels refer to the 'open' channel populated by atoms which are identical ultra-cold bosons of mass m , and to the 'closed' channel where fundamentals entities are couples of two tightly bound atoms that we here call 'molecules'. The model takes a simple form in the second quantized form, where the operator $a_{\mathbf{k}}$ annihilates an atom in the open channel with momentum \mathbf{k} , while $b_{\mathbf{k}}$ annihilates a molecule of wavevector \mathbf{k} in the closed channel. Both $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ obey standard bosonic commutation rules $[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = [b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}')$, corresponding to the choice $\langle \mathbf{r} | \mathbf{k} \rangle = \exp(i\mathbf{k} \cdot \mathbf{r})$ for the plane wave state. Any other commutator vanishes. The Hamiltonian is similar to the ones introduced for two-component or fully polarized fermions in Refs. [10, 11]:

$$\begin{aligned}
 H = & \int \frac{d\mathbf{k}}{(2\pi)^3} \left[\epsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \left(\frac{\epsilon_{\mathbf{k}}}{2} + E_{\text{mol}} \right) b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \right] \\
 & + \frac{g_0}{2} \int \frac{d\mathbf{k} d\mathbf{K} d\mathbf{k}'}{(2\pi)^9} \chi_{\mathbf{k}}^* \chi_{\mathbf{k}'} a_{\frac{\mathbf{k}}{2} - \mathbf{k}'}^\dagger a_{\frac{\mathbf{k}}{2} + \mathbf{k}'}^\dagger a_{\frac{\mathbf{K}}{2} + \mathbf{k}} a_{\frac{\mathbf{K}}{2} - \mathbf{k}} \\
 & + \Lambda \int \frac{d\mathbf{k} d\mathbf{K}}{(2\pi)^6} \left(\chi_{\mathbf{k}}^* b_{\mathbf{K}}^\dagger a_{\frac{\mathbf{K}}{2} - \mathbf{k}} a_{\frac{\mathbf{K}}{2} + \mathbf{k}} + \text{h.c.} \right). \quad (1)
 \end{aligned}$$

The first two terms in Eq. (1) are the kinetic operators in the open and closed channel respectively: $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / (2m)$, and E_{mol} is the internal energy of the molecular state in the closed channel, defined with respect to the zero energy in the open channel. The magnetic tunability of the interaction strength is due to the fact that E_{mol} is an affine function of the magnetic field \mathcal{B} with the slope $\delta\mu$, where $\delta\mu$ is the difference between the magnetic moments for an atomic pair in the open and closed channel. The second line in Eq. (1) mimics the interatomic force in the open channel which is responsible for the background scattering. In a real system it is

characterized by an attractive van der Waals tail, and the van der Waals constant C_6 sets up the short range scale of this pairwise interaction: $R_{\text{vdW}} = \frac{1}{2}(mC_6/\hbar^2)^{1/4}$. In the present model, for simplicity we choose a separable interaction, with a Gaussian weight $\chi_{\mathbf{k}} = \exp(-k^2 b^2/2)$ imposing a cut-off at short distances: $b \equiv O(R_{\text{vdW}})$. The last term in Eq. (1) describes the coupling between the two channels and models the Feshbach resonance mechanism (we choose $\Lambda \in \mathbb{R}$). The inter-channel coupling is also taken into account *via* the same Gaussian weight $\chi_{\mathbf{k}}$ as in the open channel interacting term.

We now determine the different parameters of the model from measured two-body properties. For this purpose we solve the two-body scattering problem in the center of mass frame. For an incident plane wave of energy $E = \hbar^2 k_0^2/m$ and momentum \mathbf{k}_0 , the two-body state is a coherent superposition of one molecule plus two atoms: $|\Psi\rangle = (\beta b_0^\dagger + \int \frac{d\mathbf{k}}{(2\pi)^3} A_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger)|0\rangle$, where $A_{\mathbf{k}}$ is the atomic wave function in the form:

$$A_{\mathbf{k}} = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}_0) + \frac{4\pi\hbar^2}{m} \frac{f(E)}{2\epsilon_{\mathbf{k}} - E - i0^+}, \quad (2)$$

and $f(E)$ is the scattering amplitude. Remarkably, the s -wave scattering length (denoted by a) obtained in this two-channel model can be *exactly* identified with the following expression which is known to be very accurate in the vicinity of a Feshbach resonance [12]:

$$a = a_{\text{bg}} \left(1 - \frac{\Delta\mathcal{B}}{\mathcal{B} - \mathcal{B}_0} \right). \quad (3)$$

In Eq. (3), a_{bg} is the background scattering length, and $\Delta\mathcal{B}$ is the width of the resonance located at the magnetic field \mathcal{B}_0 . One finds $a_{\text{bg}} = b g_0 \sqrt{\pi}/(g_0 - g_0^c)$, with $g_0^c = -4\pi^{3/2} \hbar^2 b/m$, an energy detuning from resonance $\nu = E_{\text{mol}} - 2\Lambda^2/g_0 + \delta\mu\Delta\mathcal{B}$ where $\nu = \delta\mu(\mathcal{B} - \mathcal{B}_0)$ and a resonance width $\Delta\mathcal{B} = 8\pi\hbar^2 \Lambda^2 a_{\text{bg}}/(m g_0^2 \delta\mu)$. This last relation implies that the energy width $\delta\mu\Delta\mathcal{B}$ always has the same sign as the background scattering length a_{bg} . We checked that this property is indeed verified for the various resonances reported in Ref. [12]. Using these parameters, the scattering amplitude admits a simple expression for $E = -\hbar^2 q^2/m < 0$ ($k_0 = iq$ and $q > 0$):

$$\frac{1}{f(E)} = q \text{erfc}(qb) - \frac{e^{-q^2 b^2}}{a_{\text{bg}}} \left(1 - \frac{\delta\mu\Delta\mathcal{B}}{E - \nu + \delta\mu\Delta\mathcal{B}} \right). \quad (4)$$

We use experimental or theoretical spectroscopic data on the two-body bound states as a way to choose a precise value for b (in absence of such data, we arbitrarily set $b = R_{\text{vdW}}$). In order to avoid any confusion the two-body bound states are denoted by 'dimers' and are distinct from the molecular state. Their binding energies $E = -E_{\text{dim}} = -\hbar^2 q_{\text{dim}}^2/m < 0$ are poles of $f(E)$. In what follows, we briefly sketch their spectrum as a function of the energy detuning ν . For $\nu < 0$, there is a branch terminating at zero energy for $\nu = 0^-$: this branch results from the interchannel coupling and is denoted below as the Feshbach dimer's branch. Furthermore, in the

case $a_{\text{bg}} > b\sqrt{\pi}$, another branch exists for all possible values of the detuning. Away from the Feshbach resonance and for $\nu > 0$, it results from the direct coupling in the open channel and we denote it as the 'background dimer' branch. For decreasing values of ν there is an avoided crossing between the two branches. We checked for several resonances that a choice of b of the order of R_{vdW} permits to describe the lowest dimer's branch over a wide range of magnetic field detuning. In Fig. (1), we compare the results of the model with the experimental data of the resonance located at $\mathcal{B}_0 \sim -11.7$ G for Cæsium [8, 9] ($\Delta\mathcal{B} \simeq 28.7$ G, $a_{\text{bg}} \simeq 1720a_0$, $R_{\text{vdW}} \simeq 101a_0$ and $\delta\mu \simeq 2.3|\mu_B|$ [12]). The system is in the vicinity of a shape resonance ($a_{\text{bg}} \gg R_{\text{vdW}}$) and the spectrum displayed corresponds to the branch of the background dimer. We found very good agreement for $b = 0.7R_{\text{vdW}}$.

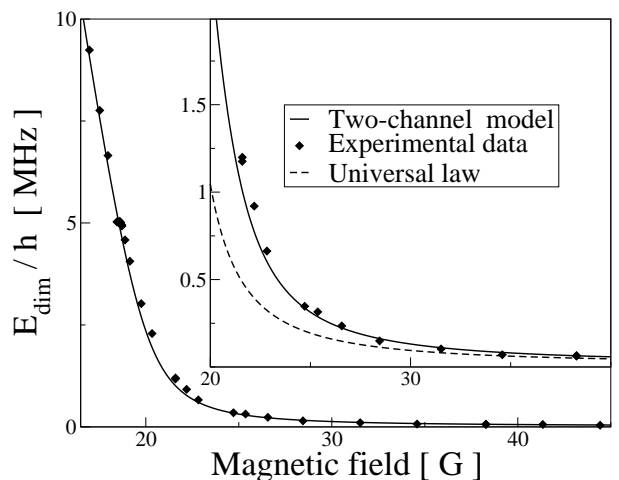


FIG. 1: Comparison between experimental dimer's energies in ^{133}Cs obtained at Innsbruck (black losanges) [8] and results of the two-channel model for $b = 0.7R_{\text{vdW}}$ (black line). Inset: detail of the deviation of the spectrum from the universal law $E_{\text{dim}} = \hbar^2/(ma^2)$ (dashed line).

We now turn to the central part of the present work by investigating the problem of three interacting bosons. The general three-body eigenstate of Eq. (1) of energy E in the total center of mass frame, is a coherent superposition of three atoms plus one atom and one molecule:

$$|\Psi\rangle = \int \frac{d\mathbf{K}}{(2\pi)^3} \frac{d\mathbf{k}}{(2\pi)^3} A_{\mathbf{K},\mathbf{k}} a_{\frac{\mathbf{K}}{2}+\mathbf{k}}^\dagger a_{\frac{\mathbf{K}}{2}-\mathbf{k}}^\dagger a_{-\mathbf{K}}^\dagger |0\rangle + \int \frac{d\mathbf{K}}{(2\pi)^3} \beta_{\mathbf{K}} b_{\mathbf{K}}^\dagger a_{-\mathbf{K}}^\dagger |0\rangle. \quad (5)$$

In Eq.(5) $A_{\mathbf{K},\mathbf{k}}$ and $\beta_{\mathbf{K}}$ are respectively the atomic and the atom-molecule wavefunctions. For $E > 0$, the atomic wavefunction contains an eigenstate of the atomic kinetic operator $A_{\mathbf{K},\mathbf{k}}^{(0)}$, and for all $E \in \mathbb{R}$, $A_{\mathbf{K},\mathbf{k}}$ can be written as:

$$A_{\mathbf{K},\mathbf{k}} = A_{\mathbf{K},\mathbf{k}}^{(0)} + \Lambda \chi_{\mathbf{k}} \beta_{\mathbf{K}}^{\text{eff}} / (E_{\text{rel}} - 2\epsilon_{\mathbf{k}} + i0^+), \quad (6)$$

where $E_{\text{rel}} = \hbar^2 k_{\text{rel}}^2/m = E - 3\hbar^2 K^2/(4m)$ is the relative energy between a pair of atoms and the third atom. For convenience, we introduced in Eq. (6) the effective atom-molecule wavefunction $\beta_{\mathbf{K}}^{\text{eff}}$:

$$\beta_{\mathbf{K}}^{\text{eff}} = \beta_{\mathbf{K}} \times (E_{\text{rel}} - \nu + \delta\mu\Delta\mathcal{B}) / (E_{\text{mol}} - \nu + \delta\mu\Delta\mathcal{B}). \quad (7)$$

The three-boson problem for this model is solved by finding the solutions of the integral equation which is deduced from the stationary Schrödinger equation:

$$\frac{m|\chi_{\mathbf{k},\text{rel}}|^2\beta_{\mathbf{K}}^{\text{eff}}}{4\pi\hbar^2 f(E_{\text{rel}})} - 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\beta_{\mathbf{k}}^{\text{eff}} \chi_{\frac{\mathbf{K}}{2}+\mathbf{k}}^* \chi_{\mathbf{K}+\frac{\mathbf{k}}{2}}}{\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{K}} + \epsilon_{\mathbf{K}+\mathbf{k}} - E - i0^+} = - \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\chi_{\mathbf{k}}^*}{\Lambda} \left(A_{\mathbf{K},\mathbf{k}}^{(0)} + 2A_{-\frac{\mathbf{K}}{2}+\mathbf{k}, -\frac{3\mathbf{K}}{4}-\frac{\mathbf{k}}{2}}^{(0)} \right). \quad (8)$$

Remarkably all the two-body physics, contained in the scattering amplitude $f(E)$, appears in the diagonal part of Eq. (8). Nearby a resonance, in the limit where $|a| \rightarrow \infty$, Eq. (8) converges asymptotically in the low-energy regime (*i.e.* for $kb \ll 1$ and $Kb \ll 1$) toward the so-called Skorniakov Ter-Martirosian equation of Ref. [13], while the high energy limit of the integral kernel acts as an ultra-violet cut-off and the Thomas collapse is avoided [14]. As the magnetic detuning $|\mathcal{B} - \mathcal{B}_0|$ is increased, off-resonant effects come into play and the model can be used to quantify deviation from the universal theory [3, 4]. To this end, we numerically solved Eq. (8) using two independent codes for several Feshbach resonances. We report in the following our results concerning the resonances studied experimentally in Refs. [1, 2, 5, 9]. First, we investigate the spectrum of trimers made of

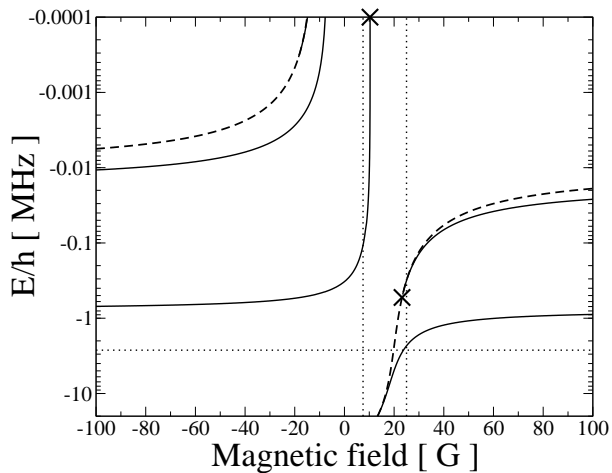


FIG. 2: Spectrum of bound states in ^{133}Cs ($\mathcal{B}_0 \sim -11.7$ G). Solid lines: trimers; dashed line: dimers; dotted horizontal line: “High energy” limit $-\hbar^2/(mR_{\text{vdW}}^2)$; dotted vertical lines: position of the Efimov resonances observed in the experiment (at 7.5 G and 25 G resp.); Crosses: thresholds computed with the two-channel model (at 10.3 G and 23.2 G resp.).

Cæsium atoms for the Feshbach resonance at -11.7 G. Trimers are obtained by searching negative energy solutions (or $E < -E_{\text{dim}}$ if a shallow dimer exists) of Eq. (8)

where $A^{(0)} = 0$. At resonance ($\nu = 0$), we recover the Efimov spectrum: $E_n = E_0 e^{-2\pi n/s_0}$, ($n \in \mathbb{N}$) where E_0 is the energy of the lowest Efimov state [of the order of $-\hbar^2/(mR_{\text{vdW}}^2)$] and $s_0 = 1.00624$ [3, 4]. In Fig. (2) we plot the spectrum as a function of the magnetic field. Our model predicts four important features: (i) The existence of two Efimov branches extending in the regions of positive and negative \mathcal{B} . Each branch is continuous through the formal limit $|\mathcal{B}| = \infty$. Other Efimov branches are located in a small interval near \mathcal{B}_0 ; (ii) The threshold of the first Efimov branch at 10.3 G observed in Ref.[5] at 7.8 G; (iii) The two trimer branches hit the background dimer branch in a non universal region where short range details of the interatomic forces are not negligible –see inset of Fig.(1)– and where our model gives qualitative informations only; (iv) In experiments reported in Ref. [9], the magnetic field was decreased from a large detuning and an atom-dimer resonance loss was found at ~ 25 G. The present model shows that the observed threshold corresponds to the second trimer branch. The disagreement between theoretical and experimental thresholds follows from item (iii). Moreover the asymptotic behavior of the wave function at distances $r \ll a$ is a crucial ingredient in Universal Theory and follows from taking the ‘unitary approximation’ of the scattering amplitude $f \sim -1/ik$ at intermediate momentum $1/a \ll k \ll \min(1/R_{\text{vdW}}, 1/r_e)$, where r_e is the effective range. However, at the observed threshold ~ 25 G, $a/R_{\text{vdW}} \sim 4$ and from Eq. (4), $a/r_e \sim 2$. Hence, in this detuning region there is no clear separation of momentum scale and the ‘unitary approximation’ for intermediate momentum is not correct. This fact gives an important insight in the deviation from prediction of Ref. [4] concerning the ratio between the scattering lengths at the two observed thresholds.

In this last part, we study the recombination of three incoming atoms of vanishing total energy into one two-body bound state and one atom. This is the main process responsible for the short life time of a resonant BEC in a dipolar trap. Experimentally, it is measured *via* the atomic loss rate which is defined for N atoms trapped in a cubic box of size L by:

$$\dot{N} = -\alpha_{\text{rec}} N(N-1)(N-2)/L^6, \quad (9)$$

where α_{rec} is the three-body recombination constant. The atomic loss rate plotted as a function of the magnetic field detuning exhibits a large peak centered at the resonance. We limit our analysis to the standard regime where for a given detuning there exists at most one shallow dimer only (a_{bg} is of the order of R_{vdW} or negative). There are two distinct regimes in the recombination process: (a) In the regime of negative energy detuning ($\nu < 0$) the formation rate of Feshbach dimers is the dominant loss mechanism. This dimer is an eigenstate of the model Hamiltonian in Eq. (1) and the recombination constant can be computed *exactly*; in what follows, it is denoted by $\alpha_{\text{rec}}^{\text{Fesh}}$; (b) In the regime $\nu > 0$ there is no shallow dimer and the deep bound states populated in inelastic scattering processes are not described by our model

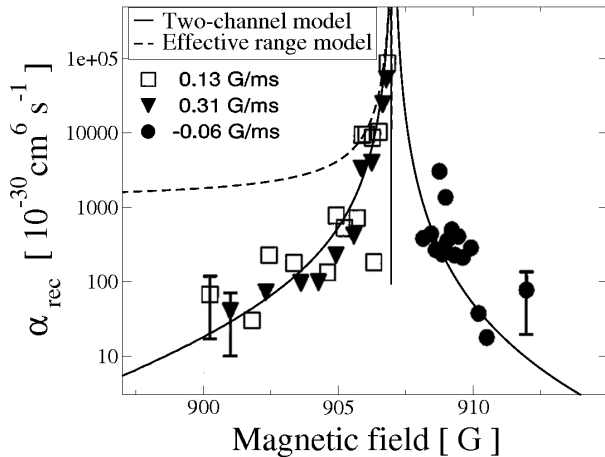


FIG. 3: Three-body recombination constant α_{rec} as a function of the magnetic field B for the narrow Feshbach resonance in ^{23}Na at 907 G. The three different symbols correspond to different ramp speeds of the magnetic field across the resonance in Ref. [2]. Solid line: prediction of the two-channel model, dashed line: prediction of the effective range model in Ref. [6]. The vertical line at resonance is due to the existence of narrow oscillations of α_{rec} also predicted in Refs. [6, 7].

Hamiltonian. In this case, we denote the recombination constant by $\alpha_{\text{rec}}^{\text{deep}}$. In both regimes the source term in Eq.(6) is $A_{\mathbf{K},\mathbf{k}}^{(0)} = (2\pi)^6 \delta(\mathbf{K})\delta(\mathbf{k})$ and corresponds to the incoming atomic wave function in the three-body scattering process. In the first regime [case (a)], the outgoing dimer and atom created by inelastic scattering have a relative momentum $\frac{2}{\sqrt{3}}q_{\text{dim}}$. The dimer formation manifests itself as an outgoing wave in the atom-molecule wave function, and the wave function $\beta_{\mathbf{K}}$ has a pole at $K = \frac{2}{\sqrt{3}}q_{\text{dim}} + i0^+$; we denote the residue of this pole by γ . In order to evaluate $\alpha_{\text{rec}}^{\text{Fesh}}$, we enclose the three incoming atoms in a fictitious box of arbitrary large size L and impose periodic boundary conditions. The wave function is then deduced from Eq. (5) with $|\Psi^{\text{box}}\rangle \simeq |\Psi\rangle/L^{9/2}$. The rate of molecule formation is obtained in configuration space by computing the total flux of the probability current associated with the atom-molecule wave function (relative particle of reduced mass $2m/3$) through the box surface. Since the flying dimer has a non vanishing probability (p_{closed}) to be in the closed channel, we di-

vide this total flux by p_{closed} thus obtaining the atomic loss rate \dot{N} . By comparing this expression with the case $N = 3$ in Eq. (9), one obtains:

$$\alpha_{\text{rec}}^{\text{Fesh}} = 2\sqrt{3}\hbar q_{\text{dim}}^3 |\gamma|^2 / (9\pi m p_{\text{closed}}). \quad (10)$$

In the regime $\nu > 0$ [case (b)], the recombination rate can be evaluated on a qualitative basis only. The idea is to compute in the fictitious box of size L the probability $\mathcal{P}_{<}$ of finding the three atoms or the atom and the molecule in a volume of the order of R_{vdW}^3 . This calculation is performed in configuration space by using Eq. (5). Since R_{vdW} gives the typical size of deep bound states, the loss rate is obtained by dimensional analysis with $\dot{N} \propto -\frac{\hbar \mathcal{P}_{<}}{m R_{\text{vdW}}^2}$, and finally the recombination constant is estimated by: $\alpha_{\text{rec}}^{\text{deep}} = \frac{\hbar L^6 \mathcal{P}_{<}}{m R_{\text{vdW}}^2}$. We applied this formalism for the narrow resonance [*i.e.* $\delta\mu\Delta B \ll \frac{\hbar^2}{ma_{\text{bg}}^2}$]

in ^{23}Na at $B_0 \simeq 907$ G [1] ($\Delta B \simeq 1$ G, $\delta\mu \simeq 3.8|\mu_B|$, $a_{\text{bg}} \simeq 63a_0$ and $R_{\text{vdW}} \simeq 44.5a_0$ [12]). Fig. (3) shows a dramatic agreement of our results (for $b = R_{\text{vdW}}$) with the experiments in Ref. [2]. Three-body properties in narrow resonances are usually described within the effective range approximation by using the two parameters a and $R^* = \hbar^2/(ma_{\text{bg}}\delta\mu\Delta B)$ [6]. As shown in Fig. (3), this latter approach gives reasonable results very close to the resonance only. In the zero range limit ($b \rightarrow 0$), when the parameters a and R^* are held fixed, and $a_{\text{bg}} \equiv 0(b)$ vanishes (but $a_{\text{bg}} \neq b\sqrt{\pi}$), the present model coincides with the effective range approach *exactly*. Therefore, in realistic situations where b and a_{bg} are both finite, this two-channel model quantifies consistently off-resonant effects. We verified that α_{rec} in Fig. (3) is not very sensible to the precise choice for $b \equiv 0(R_{\text{vdW}})$, showing that for a narrow resonance the present model gives quantitative results for the deviation from universality.

To conclude, we presented a rather simple formalism to capture the main physical features in resonant three-bosons systems. The short range details of interatomic forces are described by one parameter only, so that we avoided the complexity of more detailed models [15, 16].

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