Pseudopotential Analog for Zero-Range Photoassociation and Feshbach Resonance

M. G. Moore

Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA

A zero-range approach to atom-molecule coupling is developed in analogy to the Fermi-Huang pseudopotential approach to collisions. It is shown by explicit comparison to an exactly solvable finite-range model that replacing the molecular bound-state wave function with a regularized delta function can reproduce the exact scattering amplitude in the long-wavelength limit. Using this approach, we find an analytical solution to the two-channel Feshbach resonance problem for two atoms in a spherical harmonic trap, highlighting the strong dependence of the effective scattering length and bare-molecule population on the atom-molecule coupling strength.

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Coupling between atoms and molecules in quantum-degenerate gases is an ever-present aspect of ultracold atomic physics. Feshbach resonances (FR) [1] are now routinely used for control over atomic interactions [2] and the formation of molecular Bose-Einstein condensates [3–6]. Laser-induced photoassociation (PA) is also widely employed [7,8], having the advantage of control over both the coupling strength [9] and detuning, which depend on the laser intensity and frequency, respectively. In contrast, for FR changing the intensity of a static *B* field adjusts the detuning, while the coupling strength depends only on atomic parameters. While a pseudopotential [10] approach to atom-atom collisions has long been a cornerstone of Bose-Einstein condensation (BEC) theory, an analog has yet to be formulated to treat multichannel free-bound coupling in ultracold atomic gases. In this Letter, we formulate such an approach which is applicable to both the FR and PA versions of atom-molecule coupling.

The first zero-range models for BEC atom-molecule coupling replaced the bound-state wave function with a simple delta function [11–14]. While suitable for mean-field models, the delta function model is known to introduce a UV divergence when atom-atom correlations are taken into account. A renormalization scheme was developed by Holland and co-workers [15], where the divergence is removed via a momentum cutoff and a cutoff-dependent shift to the bound-state energy. In subsequent work, this approach was extended to include zero-range atom-atom collisions by introducing cutoff-dependent renormalized coupling constants [16].

The origin of the UV divergence lies in "rogue dissociation" [17,18] of molecules into "virtual" atom pairs, which form a $1/r$ core in the relative wave function of a pair of atoms which necessarily exists in superposition with any bound-state amplitude. A zero-range approach involves replacing the molecular bound state with a zero-range object, which sits at the center of this core; hence, a simple delta function leads to a nonphysical divergence. In this work, we show that if the correct zero-range object is employed, the long-wavelength scattering properties of a finite-range model can be exactly reproduced without in-

troducing renormalized (infinite) detunings and or coupling constants. The correct zero-range pseudowave function is a regularized delta function, whose (finite) coefficient depends only on the details of the interatomic potential. We note that the renormalization approach of Ref. [16] is not as desirable in the presence of a trapping potential, because the renormalized parameters must then depend not just on the cutoff but also on the relative energy of each atom pair. The present approach contains no energy-dependent parameters or explicit momentum cutoff and can be considered as a closed-form analytic expression for the cutoff $\rightarrow \infty$ limit of the previous renormaliztion approach.

We proceed by first analyzing a model square-potential system and establishing the validity of the regularized delta function approach. We then obtain an analytic solution for the 2-atom problem in a harmonic trap. We examine the dependence of the effective scattering length and bare-molecule populations on the coupling strength and detuning. Our primary result is to demonstrate that the bare-molecule population decreases as the square of the coupling strength, a result qualitatively consistent with similar recent results [19,20]. This suggests that PA is a more versatile tool than FR for control over atom-molecule coupling.

We begin our analysis by considering a pair of atoms described by a relative wave function $\phi_j(\mathbf{r}, t)$, where $j = 1, 2$ corresponds to an internal spin state. The eigenstates of this system obey the Schrödinger equation

$$E\phi_j(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\nabla^2\phi_j(\mathbf{r}) + \sum_k V_{jk}(\mathbf{r}, t)\phi_k(\mathbf{r}), \quad (1)$$

where E is the energy eigenvalue, μ is the reduced mass, and $V_{jk}(\mathbf{r})$ is the interatom potential. For our model system, we assume that the first channel sees a flat potential, $V_{11}(\mathbf{r}) = 0$. The second channel sees a spherical-well potential of depth V_0 and radius w, $V_{22}(\mathbf{r}) = U_0 - V_0 U(w - r)$, where U_0 is the continuum threshold energy and $U(x)$ is the unit-step function. In the absence of coupling terms, the spectrum of the second channel consists of a continuum of

states above the threshold energy U_0 and a discrete set of bound states with energies between U_0 and $U_0 - V_0$. The bound states are all of the form

$$\psi_b(\mathbf{r}) = \begin{cases} \mathcal{N}_b \dfrac{e^{-r/a_b}}{r} & r > w \\ \mathcal{N}_b \dfrac{e^{-w/a_b}}{\sin(k_b w)} \dfrac{\sin(k_b r)}{r} & r < w, \end{cases} \quad (2)$$

where a_b and k_b satisfy the equations $(\hbar^2/2\mu) \times [k_b^2 + 1/a_b^2] = V_0$ and $\cot(k_b w) = -1/(k_b a_b)$, and $\mathcal{N}_b$ is determined by normalization.

We proceed by first expanding the second channel wave function $\phi_2(\mathbf{r})$ onto its bare eigenstates under the simplifying assumptions that only a single bound state is near-resonantly coupled to the first channel so that all other states may be neglected. We assume the interaction potential has the form $V_{12}(\mathbf{r}, t) \approx (\hbar^2 G/\mu)e^{-i\omega t}$. Taking $E = \hbar^2 k^2/(2\mu)$ then leads to an eigenvalue problem for a continuum coupled to a single bound state,

$$\tfrac{1}{2}[k^2 + \nabla^2]\phi_1(\mathbf{r}) = G\psi_b(\mathbf{r})c, \quad (3)$$

$$\frac{1}{2}[k^2 - 2\Delta]c = G^* \int d^3 r \psi_b^*(\mathbf{r})\phi_1(\mathbf{r}), \quad (4)$$

where c is the probability amplitude for the atom pair to be in the bound state, and $\Delta = (\mu/\hbar^2)(U_0 - \omega) - (1/2a_b^2)$ is the detuning away from the atom-molecule resonance at $k = 0$. The coupling constant G will depend on the details of the atom-molecule coupling scheme.

Our goal is now to solve this eigenvalue problem, under the boundary conditions $\lim_{r\to\infty}\phi_1(\mathbf{r}) = (e^{-ikr}/r) + f(e^{ikr}/r)$ and $\lim_{r\to 0}r\phi_1(\mathbf{r}) = 0$, in order to determine the scattering amplitude $f = f(k)$. The solution can be obtained via the ansatz

$$\phi_1(\mathbf{r}) = \begin{cases} \dfrac{e^{-ikr}}{r} + f\dfrac{e^{ikr}}{r} + \dfrac{2Ga_b^2}{1+(a_b k)^2}c\psi_b(\mathbf{r}) & r > w \\ \beta\dfrac{\sin(kr)}{r} + \dfrac{2G}{k^2-k_b^2}c\psi_b(\mathbf{r}) & r < w. \end{cases} \quad (5)$$

This ansatz explicitly satisfies (3), as well as the boundary conditions. Equation (4), together with the continuity equations $\phi_1(w^+) = \phi_1(w^-)$ and $\nabla\phi_1(w^+) = \nabla\phi_1(w^-)$, can then be used to determine the three unknowns f, c, and β.

The long-wavelength limit requires that $1/k$ be large compared to the size of the bound state. As the size of the bound state is $w + a_b$, this is equivalent to the limits $kw \ll 1$ and $ka_b \ll 1$. For our model potential, the condition $K_b > 1/w$ is always satisfied, so that k/K_b is a small parameter as well. Expanding the scattering amplitude $f(k)$ in terms of these small parameters then yields

$$f(k) = -\frac{k^2 - 2\delta - ik\frac{|\chi|^2}{\pi}}{k^2 - 2\delta + ik\frac{|\chi|^2}{\pi}} + O[\varepsilon^3], \quad (6)$$

where $\varepsilon \in \{kw, ka_b, k/K_b\}$, and we have introduced the light-shifted detuning

$$\delta = \Delta - 8\pi|G|^2\mathcal{N}_b^2 e^{-2w/a_b}\left[\frac{e^{2w/a_b}}{\mathcal{N}_b^2 K_b^2} - \left[1 + \frac{1}{K_b^2 a_b^2}\right]\frac{a_b^3}{2}\right.$$
$$\left. + \left[1 + \frac{1}{K_b^2 a_b^2}\right]^2 a_b^2(a_b + w)\right], \quad (7)$$

and the effective coupling constant

$$\chi = 4\pi G\mathcal{N}_b e^{-w/a}a_b(a_b + w)\left[1 + \frac{1}{K_b^2 a_b^2}\right]. \quad (8)$$

The important point here is that all of the details of the potential can be absorbed into effective detuning and coupling constants.

We now consider a zero-range model in which the bound-state wave function $\psi_b(\mathbf{r})$ in (3) is replaced by a regularized delta function via $G\psi_b(\mathbf{r}) \to \chi\delta^3(\mathbf{r})\frac{\partial}{\partial r}r$. In addition, the detuning Δ is replaced by the light-shifted detuning δ. The Schrödinger equation for this model is given by

$$\tfrac{1}{2}[k^2 + \nabla^2]\phi_1(\mathbf{r}) = \chi\delta^3(\mathbf{r})c, \quad (9)$$

$$\frac{1}{2}[k^2 - 2\delta]c = \chi^* \int d^3 r\delta^3(\mathbf{r})\frac{\partial}{\partial r}r\phi_1(\mathbf{r}). \quad (10)$$

This problem can be solved by making use of the ansazt $\phi_1(\mathbf{r}) = (e^{-ikr}/r) + f(e^{ikr}/r)$, resulting in a scattering amplitude given by Eq. (6), but without the $O[\varepsilon^3]$ correction. Thus, the zero-range model (9) and (10) will reproduce correctly the long-wavelength atom-molecule quantum dynamics of our model potential.

As an example, we now solve the problem of two bosonic atoms in a spherical harmonic oscillator (frequency ω_{trap}) with both s-wave collisions and coupling to a bound state in a second channel. With $E = \hbar\omega_{\text{trap}}(\nu_n + 3/2)$, $\delta \to \hbar\omega_{\text{trap}}\delta$, and using harmonic oscillator units, the time-independent Schrödinger equation can be written as

$$[\nu_n + \tfrac{1}{2}\nabla^2 - \tfrac{1}{2}r^2 + \tfrac{3}{2}]\phi_n(\mathbf{r}) = \kappa_n\delta^3(\mathbf{r}), \quad (11)$$

$$[\nu_n - \delta]c_n = \pi^{3/4}\Omega \int d^3 r\delta^3(\mathbf{r})\frac{\partial}{\partial r}r\phi_n(\mathbf{r}), \quad (12)$$

where n is an integer label for each quantum level (the lowest energy level corresponding to $n = 0$), a is the background scattering length, λ is the harmonic oscillator length of the trap, $\Omega = \lambda^2\pi^{-3/4}\chi$, and $\kappa_n = \pi^{3/4}\Omega c_n + 2\pi(\frac{a}{\lambda})\frac{\partial}{\partial r}r\phi_n(\mathbf{r})|_{r=0}$.

The normalized eigenfunctions are found to be [21]

$$\phi_n(\mathbf{r}) = -\frac{\Omega}{2\pi^{3/4}}\frac{\Gamma[-\frac{\nu_n}{2}]}{\beta(\nu_n, \frac{a}{\lambda})}c_n e^{-r^2/2}U\left(-\frac{\nu_n}{2}, \frac{3}{2}, r^2\right), \quad (13)$$

where $\beta(\nu, x) = 1 - 2x\Gamma[-\frac{\nu}{2}]/\Gamma[-\frac{\nu+1}{2}]$, $U(a, b, z)$ is the confluent hypergeometric function, and $\psi(z)$ is the polygamma function [22]. The eigenvalues $\{\nu_n\}$ are determined by the characteristic equation

$$\delta = \nu_n - \frac{\Omega^2 \sqrt{\pi} \Gamma[-\frac{\nu_n}{2}]}{\Gamma[-\frac{\nu_n+1}{2}]\beta(\nu_n, \frac{a}{\lambda})}. \qquad (14)$$

Intriguingly, it is found that the bare-molecule fraction $|c_n|^2$ obeys the relation $|c_n|^2 = d\nu_n/d\delta$. From a series expansion of (13), the $1/r$ part of $\phi_n(\mathbf{r})$ is found to be $-[\Omega/2\pi^{1/4}\beta(\nu_n, \frac{a}{\lambda})](c_n/r)$. Only for $a = 0$ is this term independent of ν_n, so that it can be removed via an energy-independent renormalized detuning [15].

The spectrum of eigenvalues agrees exactly with those of a single-channel system with the energy-dependent effective scattering length

$$a_{\text{eff}}(\nu) = a + \frac{\lambda}{2}\frac{\sqrt{\pi}\Omega^2}{(\nu - \delta)}, \qquad (15)$$

which is the familiar FR result. The only difference between the true atom-molecule eigenstates and the equivalent single-channel states with scattering length a_{eff} is the presence of the bare-molecule population $|c_n|^2$.

On resonance, we have $\nu_n = \delta$ and $|a_{\text{eff}}| \rightarrow \infty$. A careful analysis shows that this requires $\nu_n = 2n - 1$ and $c_n \neq 0$. Thus, the eigenvalues are driven to odd-integer values, for which the regular part of $\phi_n(\mathbf{r})$ vanishes at $\mathbf{r} = 0$. This result leads to an analytic expression for the on-resonance molecular fraction $|c_n|^2 = 1/(1 + \alpha_n\Omega^2)$, where $\alpha_n = [(2n)!!/(2n-1)!!](\pi/2)$.

The energy dependence in $a_{\text{eff}}(\nu)$ plays a crucial role in the crossover between the weak-coupling and strong-coupling regimes. The requirement for a significant deviation from the bare-trap spectrum $\tilde{\nu}_n$ is $a_{\text{eff}}/\lambda \sim 1$. Obtaining this condition via Feshbach resonance requires $|\delta - \tilde{\nu}_n| < \sqrt{\pi}\Omega^2/2$. In the weak-coupling regime $\Omega^2 \ll 1$, only one trap level can be near resonance; thus, the spectrum consists of a series of avoided crossings between the bare-molecular level and the uncoupled eigenstates of the "open" channel. This is illustrated in Fig. 1, where we have plotted the eigenvalue spectrum as a function of the detuning for the case $a = 0.3\lambda$ and $\Omega = 0.2$. The dotted lines show the uncoupled ($\Omega = 0$) eigenvalues. It is important to note that the avoided crossings do *not* correspond to the location of the Feshbach resonance. The FR

condition $\nu_n = \delta$ occurs slightly to the left of each avoided crossing, where the perturbed eigenvalue is resonant with the bound-state energy. The large avoided crossing at $\delta = -7$ occurs when the bound state in the closed channel crosses the bound state in the open channel. There is no FR associated with this crossing.

In the strong-coupling regime, defined as $\Omega^2 \gg 1$, the width of the resonance is much larger than the trap level spacing; hence, many levels can be resonant simultaneously. Thus, the low-lying levels all lie very close to their on-resonance values of $\nu_n = 2n - 1$. This is illustrated in Fig. 2, which shows the eigenvalue spectrum as a function of detuning for the case $\Omega = 10$ and $a = 0$. In this regime, the resonance value is a good estimate for the molecular fraction, showing that the molecular amplitude decreases dramatically with increasing coupling strength. To understand this effect, simply make the reasonable assumption that in the strong-coupling limit all quasiresonant levels are mixed with equal amplitudes. For $\Omega^2 \gg 1$, the number of near-resonant levels is $N_{\text{levels}} \approx \Omega^2$. If we equate the probability for any given bare state to the total probability divided by the approximate number of levels, we arrive at $|c|^2 \approx 1/\Omega^2$, which agrees well with the analytic result.

In Fig. 3, we plot a_{eff} and $|c_n|^2$ versus detuning for several cases of interest. In Figs. 3(a) and 3(b), we show the weak-coupling case $\Omega = 0.2$ and $a = 0.3\lambda$ for levels $n = 1$ and $n = 2$, respectively. The $n = 1$ case shows a sweep (right to left) from the lowest "unbound" state through the closed channel and into the bound state in the open channel. The $n = 2$ case shows a transfer from one unbound state to another via the molecular state. As the level is swept through resonance, we see a broad feature in the molecular fraction $|c_n|^2$, whose maximum value is slightly larger than the on-resonance value and occurs to the right of the resonance. Figures 3(c) and 3(d) show the intermediate case $\Omega = 1$ and $a = 0$ for levels $n = 0$ and $n = 1$. We see in the $n = 1$ case that the molecular fraction is significantly reduced compared to the weak-coupling regime. Last, in Figs. 3(e) and 3(f), we see the strong-
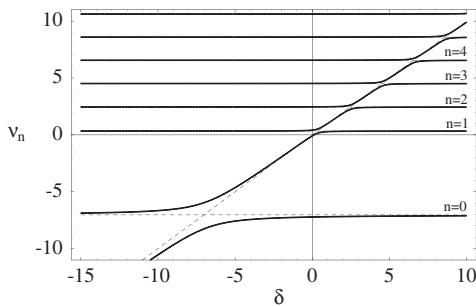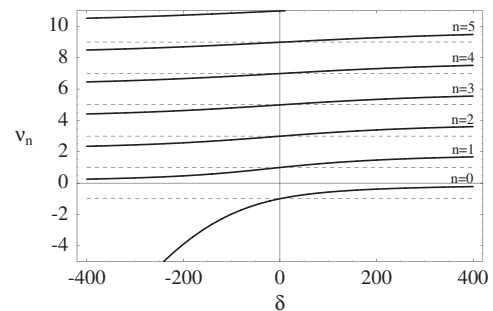

FIG. 1. Energy levels as a function of detuning for the case $a = 0.3\lambda$ and $\Omega = 0.2$, illustrating a sequence of avoided crossings in the weak-coupling regime. The dashed lines correspond to the uncoupled eigenvalues.

FIG. 2. Energy levels as a function of detuning for the case $a = 0$ and $\Omega = 10$, illustrating the "fermionization" of the low-lying levels in the strong-coupling regime (in the vicinity of $\delta = 0$). The dashed lines correspond to the odd-integer values $\nu_n = 2n - 1$.
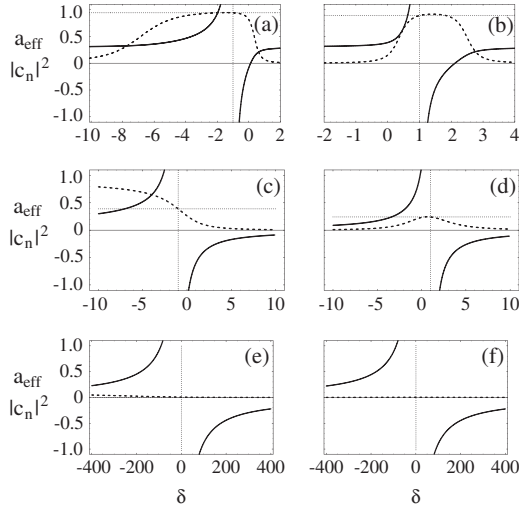
FIG. 3.   Effective scattering length a_{eff} (solid line) and molecular fraction $|c_n|^2$ (dashed line) as the detuning δ is swept across resonance. (a) and (b) show the cases $n = 1$ and $n = 2$, respectively, for the case $\Omega = 0.2$ and $a = 0.3\lambda$. (c) and (d) show $n = 0$ and $n = 1$ for $\Omega = 1$ and $a = 0$, respectively, while (e) and (f) show $n = 0$ and $n = 1$ for the case $\Omega = 10$ and $a = 0$, respectively. The vertical dotted lines mark the location of the resonance, while the horizontal dotted lines correspond to the analytical resonance result for $|c_n|^2$.

coupling case $\Omega = 10$ and $a = 0$, for levels $n = 0$ and $n = 1$. We see that, in the strong-coupling regime, the scattering length can be tuned from $-\infty$ to $+\infty$, with a negligible bare-molecular component.

In conclusion, we see that the effects of rogue dissociation play a major role in atom-molecule coupling, resulting in the appearance of a $1/r$ singularity in the relative wave function together with a corresponding decrease in the bare-molecule population. This suggests that for molecule formation it is best to have a weak coupling, while for manipulation of atomic interactions, e.g., for BCS pairing of fermions [23,24], a strong coupling will remove the corresponding bare-molecule population. In FR the free-space coupling strength is predetermined by atomic properties; hence, Ω can only be increased by decreasing the trap size. In PA, however, the coupling strength is readily increased by increasing the laser intensity. This suggests that laser-induced photoassociation may have a significant advantage over Feshbach resonance for tuning atom-atom interactions.

Last, we note recent theory work [25] in which recent fermion data [26] were successfully modeled only by employing a finite momentum cutoff, thus calling into question the validity of the zero-range approximation in the ^{6}Li system. In the present work, it was found that the zero-range approach should fail when the incident wavelength is small compared to the size of the bare bound state. At face value, this is inconsistent with the fitted cutoff length of $1500a_0$. This discrepency must be understood before applying the present pseudopotential approach to

the ^{6}Li system.

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