Universality in s-wave and higher partial wave Feshbach resonances: an illustration with a single atom near two scattering centers

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It is well-known that cold atoms near s-wave Feshbach resonances have universal properties that are insensitive to the short-range details of the interaction. What is less known is that atoms near higher partial wave Feshbach resonances also have remarkable universal properties. We illustrate this with a single atom interacting resonantly with two fixed static centers. At a Feshbach resonance point with orbital angular momentum \( L \geq 1 \), we find \( 2L + 1 \) shallow bound states whose energies behave like \( 1/R^{2L+1} \) when the distance \( R \) between the two centers is large. We then compute corrections to the binding energies due to other parameters in the effective range expansions. For completeness we also compute the binding energies near s-wave Feshbach resonances, taking into account the corrections. Afterwards we turn to the bound states at large but finite scattering volumes. For p-wave and higher partial wave resonances, we derive a simple formula for the energies in terms of a parameter called “proximity parameter”. These results are applicable to a free atom interacting resonantly with two atoms that are localized to two lattice sites of an optical lattice, and to one light atom interacting with two heavy ones in free space. Modifications of the low energy physics due to the long range Van der Waals potential are also discussed.

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I. INTRODUCTION

Cold atoms with de Broglie wave lengths that greatly exceed the range of inter-atomic potential are known to exhibit universal properties that are mainly determined by the s-wave scattering length \( a_0 \). Interactions in higher partial wave channels are usually suppressed by the centrifugal barrier, unless the atoms are near a p-wave \([1,13]\), d-wave \([14,16]\), or higher partial wave \([17,20]\) Feshbach resonances.

The universality is particularly remarkable when the atoms are near a broad \([21,22]\) s-wave Feshbach resonance, near which \( a_0 \) is large but the effective range \( r_0 \) is small \([23,24]\). For example, if \( a_0 \) is positive and large there is a shallow two-body bound state with energy entirely determined by \( a_0 \) rather than the full atomic details of the interaction \([22,26]\):

\[
E \approx -\frac{\hbar^2}{2\mu a_0^2},
\]

where \( \mu \) is the reduced mass, and \( \hbar \) is the Planck constant over \( 2\pi \). For three or more atoms with large scattering length, there is another remarkable manifestation of universality: the Efimov effect \([27,28]\); in particular, at \( a_0 = \pm \infty \), there are an infinite sequence of three-body shallow bound states whose energies form a geometric sequence with a ratio that is determined by the quantum statistics and the mass ratios of atoms \([20,22,23]\), but not affected by the details of short-range interaction \([20,28]\). There have been predictions of analogous effects in two-atom systems with large s-wave scattering length \([31]\).

Unlike the s-wave resonance, higher partial wave Feshbach resonances have not been extensively analyzed from the perspective of universality. There have been efforts to look for Efimov effect near p-wave resonances \([22,34]\), but Nishida pointed out that Efimov effect is not possible in such a case \([35]\).

In this work, we illustrate that near higher partial wave resonances, although there is no Efimov effect in three dimensions, the concept of universality remains powerful. By universality we mean that there are many physical properties controlled by one or two effective parameters for the interaction, rather than by the full atomic details. Consequently different atomic species near higher partial wave Feshbach resonances can exhibit very similar behaviors.

We study a single free atom of mass \( M \) having short-range interactions with two identical static centers. The interaction is tuned to a resonance in the \( L \)th partial wave channel. Here \( L \) is the quantum number for the relative orbital angular momentum between the atom and one center. If the \( L \)-wave scattering volume \( a_L \) is infinity, we find that there are \( 2L + 1 \) shallow bound states with energies entirely controlled by the \( L \)-wave effective range \( r_L \):

\[
E = -\frac{\hbar^2}{2M} \frac{\chi_{Lm}}{(-r_L)^{2L+1}}, \quad m = -L, -L+1, \ldots, L \quad (1)
\]

if \( L \geq 1 \). Here \( R \) is the distance between the two centers, \( m \) is the projection of orbital angular momentum along the line connecting the two centers,

\[
\chi_{Lm} = 2(2L+1)!!(2L-1)!! \left( \frac{2L}{L+m} \right), \quad (2)
\]

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and \( \binom{2L}{L + m} = \frac{(2L)!}{(L + m)!(L - m)!} \) are binomial coefficients. 

\( a_L \) and \( r_L \) are defined as parameters in the low-energy effective range expansion for the scattering phase shifts, Eq. (13). Note that \( r_L \) is negative if \( L \geq 1 \). We shall also study the bound states when \( a_L \) is large but finite in Secs. IV, V, and VI.

Even when \( a_L = \pm \infty \), there are corrections to Eq. (1) due to a nonzero radius of the interaction. Such corrections decay more rapidly at large \( R \) than the dominant term, so that at large values of \( R \) Eq. (1) becomes increasingly more accurate. We determine these corrections in Sec. III.

At the \( s \)-wave resonance \( (a_0 = \pm \infty) \), the problem of a single atom interacting with two centers has been studied in Refs. \[26, 30, 40, 42\]. It was found that the shallow binding energy

\[
E = -\frac{\hbar^2 \chi^2}{2MR^2} \tag{3}
\]

and is independent of the effective range \( r_0 \) at the leading order \[26, 30, 40, 42\]. Here \( \chi_0 \approx 0.567143 \) is the real solution to the equation \( e^{-\chi_0} = \chi_0 \). This inverse square dependence of the energy on \( R \) qualitatively explains the presence of Efimov effect for two heavy atoms interacting resonantly with a light atom. Within the Born-Oppenheimer approximation the two heavy atoms are effectively interacting via a potential equal to the light atom. Since the potential decays like \( 1/R^2 \) and is strong compared to the kinetic energy of the heavy atoms, there is a sequence of three-atom bound states with energies forming a geometric sequence \[26, 30, 40\].

For two heavy atoms interacting with a light atom near higher partial wave Feshbach resonances, Eq. (1) shows that Efimov effect is absent, in agreement with Ref. \[53\], since the effective potential induced by the light atom now decays like \( 1/R^3 \) for \( p \)-wave resonance, \( 1/R^5 \) for \( d \)-wave resonance, etc.

Despite the absence of Efimov effect, the simple power laws for the shallow bound states in Eq. (2) illustrates the elegance of universality in higher partial wave resonances.

In Sec. IV we derive a more general simple approximate formula, Eq. (4), when \( |a_L|^{-1/(2L+1)} \) and \( R \) are both large and finite.

One could experimentally confirm Eq. (1) and Eq. (4) using a light atom and two heavy atoms, or using a free atom having confinement induced scattering resonance \[43, 44\] with two other atoms pinned to two lattice sites of an optical lattice.

The outline of the rest of this paper is as follows.

In Sec. II we derive the general equations for the shallow bound states of an atom near two centers.

In Sec. III we derive large-\( R \) expansions for the bound states at resonance (\( a_L = \infty \)).

In Sec. IV we derive the \( O(1/a_L) \) corrections to the wave numbers of the bound states slightly off resonance.

In Sec. V we compute the binding energies approximately when \( |a_L|^{-1/(2L+1)} \) and \( R \) are both large and may be comparable.

In Sec. VI we derive a simple formula for the binding energies near a \( p \)-wave or higher partial wave resonance.

In Sec. VII we consider the effects of a long range Van der Waals interaction between the atom and each center.

In Sec. VIII we summarize our findings, discuss some technical limitations of this work, and argue that despite such limitations, our results will be useful in various experimental scenarios.

II. GENERAL PROPERTIES OF THE BOUND STATES

We consider an atom of mass \( M \) attracted by two fixed identical scattering centers that are separated by distance \( R \) and located along the \( z \)-axis, with Cartesian coordinates \( s_1 = (0, 0, -R/2) \) and \( s_2 = (0, 0, R/2) \). The potential experienced by the atom is assumed to vanish unless the atom is very close to one center. This idealized model is a good approximation for neutral atoms, which have a long range Van der Waals potential that decays rapidly at large distance; effects of this long range potential are discussed in Sec. VII.

Each scattering center is characterized by phase shifts \( \delta_l(k) \) where \( l = 0, 1, 2, \ldots \) is the orbital angular momentum of the atom about the center and \( k \equiv \hbar \kappa \) is the wave number. The energy of the atom is

\[
E = \frac{\hbar^2 k^2}{2M} = -\frac{\hbar^2 \kappa^2}{2M}. \tag{4}
\]

For a bound state we take \( \kappa > 0 \).

Due to the axial symmetry of the system about the \( z \) axis and the parity symmetry about the origin, we may consider bound states with a certain orbital magnetic quantum number \( m \) and a certain parity \( \sigma \in \{+, -\} \). Outside the range of potential the wave function of the atom is

\[
\psi_{m\sigma}(r) = \sum_{l = |m|}^{\infty} C_{l}^{m\sigma} \left[ h_l^{(1)}(ikr_1)Y_{lm}(\hat{r}_1) + \sigma(-1)^l h_l^{(1)}(ikr_2)Y_{lm}(\hat{r}_2) \right], \tag{5}
\]

which satisfies

\[
\psi_{m\sigma}(-r) = \sigma \psi_{m\sigma}(r). \tag{6}
\]

Here \( r \) is the position vector of the atom, \( r_{\alpha} \equiv r - s_{\alpha} \) is the position vector of the atom relative to a center, \( \hat{r}_{\alpha} \equiv r_{\alpha}/r_{\alpha} \), and \( Y_{lm} \) is the spherical harmonic, and \( h_l^{(1)}(x) \) is the spherical Hankel function of the first kind. The coefficients \( C_{l}^{m\sigma} \) and the parameter \( \kappa \) should be chosen such that in the vicinity of a center located at \( s_{\alpha} \) (\( \alpha =
1, 2) the wave function takes the form:

\[ \psi_{m\sigma}(r) = \sum_{l=|m|}^{\infty} C_{l\sigma}^{m} \left[ j_l(kr) \cot \delta_l(k) - n_l(kr) \right] Y_{lm}(\hat{r}_\alpha), \tag{7} \]

where \( j_l(x) \) and \( n_l(x) \) are the spherical Bessel functions of the first kind and the second kind, respectively. Because of the well-defined parity, we need to impose condition

\[ F_{ll'}^{m}(r) = \sum_{j=0}^{\text{min}(l,l')-m} \frac{j!(2j+2m-1)!}{(j+2m)!} \binom{l-m}{j} \binom{l'-m}{j} Y_{ll'}^{m}(\hat{r}_1). \tag{9} \]

Comparing the above formula with the required form of the expansion of the wave function in Eq. (7), we find

\[ \psi_{m\sigma}(r) = \sum_{l=|m|}^{\infty} \left\{ C_{l\sigma}^{m} + \sum_{l'=|m|}^{\infty} \sigma C_{l'\sigma}^{m} F_{ll'}^{m}(\kappa R) \right\} j_l(ikr_1) \tag{10} \]

and \( \frac{n!}{j!(n-j)!} \) is the binomial coefficient. Substituting the identities \( h_l^{(1)}(x) = j_l(x) + in_l(x) \) and Eq. (5), and noting that \( F_{ll'}^{m}(r) = F_{ll'}^{m}(x) \), we find

\[ h_l^{(1)}(ikr_1) Y_{lm}(\hat{r}_2) = (-1)^{l+1} \sum_{l'=|m|}^{\infty} F_{ll'}^{m}(\kappa R) j_{l'}(ikr_1) Y_{l'm}(\hat{r}_1), \tag{8} \]

where

\[ h_l^{(1)}(ikr_1) = \frac{(2l+1)(2l'+1)(l+m)(l'+m)}{(l-m)!(l'-m)!} \frac{h_l^{(1)}(ix)}{(-ix)^{m+j}}, \tag{9} \]

If \( \sigma(-1)^m = -1 \), the wave function vanishes on the \( xy \) plane, and the energy is the same as we would obtain by imposing a hard wall potential there; thus the closer the two centers, the closer the hard wall is to one center, and the higher the energy, hence the energy increases as we reduce the distance between the two centers. In the language of the chemical bond theory, the state with parity \( \sigma = (-1)^{m+1} \) may be called an anti-bonding state. We have also verified numerically that for \( \sigma = (-1)^m \), for which the wave function is an even function of \( z \), the energy decreases as we reduce the distance between the two centers; see Sec. III. Thus

\[ \sigma = \begin{cases} (-1)^m, & \text{for bonding states,} \\ (-1)^{m+1}, & \text{for anti-bonding states.} \end{cases} \tag{15} \]

For a particular \( m \), depending on the interaction between the atom and the centers and the distance \( R \) between the two centers, the atom may have two shallow bound states one from each parity, or a single shallow bound state with \( \sigma = (-1)^m \), or no shallow bound state. More details will be shown in Sec. III.
At an s-wave resonance,

\[
\kappa = \frac{0.567143}{R} \left[ 1 + \frac{0.180948 r_0}{R} + \frac{0.0688446 r_0^2}{R^2} + \frac{-2.66638 a_1 + 0.0332811 r_0^3}{R^3} - 0.00485019 r_0' \right]
+ \frac{-0.865928 a_1 r_0 + 0.0181467 r_0^4}{R^4} - 0.00544592 r_0 r_0'
+ \frac{(-45.6556 a_2 - 0.473306 a_1 r_0^2 + 0.0106396 r_0^3 - 0.00483849 r_0^2 r_0' - 0.0000520023 r_0'' + 0.428823 a_1 r_1) + O\left(\frac{1}{R^6}\right)}{R^5},
\]

(16)

The leading order term in the above series is consistent with previous theoretical calculations \[26, 30, 40–42\]. The binding energy \(E\) has the \(-1/R^2\) dependence, which leads to the emergence of three-body Efimov states. Moreover, the effects of the parameters \(r_0, r_0', r_0''\) etc in the effective range expansion Eq. (13) appear only in higher order terms. Also, the effects of other partial wave channels are all higher order corrections. In this sense, the resonant partial wave channel is dominant, in agreement with our intuition.

The results at \(p, d, f\)-wave resonances are listed in the following.

1. For \(p\)-wave resonance:

(a) \(m = 0\),

\[
\kappa = \frac{\sqrt{12}}{\sqrt{-r_1}} R^{3/2} \left[ 1 - \frac{a_0}{4R} \right] + \frac{288 - 96 a_0 r_1 + 7 a_0^2 r_1^2}{32 r_1^2 R^2} \frac{\sqrt{3} (36 - 20 a_0 r_1 + 5 a_0^2 r_1^2)}{5 (-r_1)^{3/2} R^{5/2}}
+ \frac{-1536 - 864 a_0 r_1 + 288 a_0^2 r_1^2 - 25 a_0^3 r_1^3 - 64 r_1 r_1'}{128 r_1^2 R^3}
- \frac{\sqrt{3} (180 + 924 a_0 r_1 - 595 a_0^2 r_1^2 + 70 a_0^3 r_1^3)}{35 (-r_1)^{3/2} R^{5/2}}
+ O\left(\frac{1}{R^4}\right)];
\]

(17)

(b) \(m = \pm 1\),

\[
\kappa = \frac{\sqrt{6}}{\sqrt{-r_1}} R^{3/2} \left[ 1 + \frac{3}{2 r_1 R} \right] + \frac{2 \sqrt{6}}{(-r_1)^{3/2} R^{3/2}} + \frac{9}{8 r_1^2 R^2} - \frac{57 \sqrt{6}}{5 (-r_1)^{3/2} R^{5/2}} + \frac{1083 + 4 r_1 r_1'}{16 r_1^2 R^3} + \frac{1521 \sqrt{6}}{70 (-r_1)^{3/2} R^{5/2}} + O\left(\frac{1}{R^4}\right)].
\]

(18)

2. For \(d\)-wave resonance:

(a) \(m = 0\),

\[
\kappa = \frac{\sqrt{540}}{\sqrt{-r_2}} R^{5/2} \left[ 1 - \frac{a_0}{12 R} \right] + \frac{23 a_0}{288 R^2} + \frac{-265 a_0}{3456} - \frac{9 a_1}{4 R^2} + \frac{15}{r_2} - \frac{\sqrt{3} 15 a_0^2}{\sqrt{-r_2} R^{7/2}} + \frac{12235 a_3}{16588} + \frac{21 a_0 a_1}{16} - \frac{65 a_0}{4 R^2} + O\left(\frac{1}{R^{9/2}}\right)];
\]

(19)

(b) \(m = \pm 1\),

\[
\kappa = \frac{\sqrt{360}}{\sqrt{-r_2}} R^{5/2} \left[ 1 - \frac{-9 a_1}{R^3} + \frac{15 r_2'}{R^3} \right] - \frac{15 r_2'}{r_2^2 R^6} + \frac{27 (1600 - 720 a_1 r_2 + 13 a_1^2 r_2^2)}{128 r_2^2 R^6} - \frac{39375 a_3}{4 R^7}
- \frac{45 (36 a_1^2 r_1 r_2 + 200 r_2' - 9 a_1 r_1 r_2')}{8 r_2^3 R^8} + O\left(\frac{1}{R^9}\right)];
\]

(20)

(c) \(m = \pm 2\),

\[
\kappa = \frac{\sqrt{90}}{\sqrt{-r_2}} R^{5/2} \left[ 1 + \frac{15}{2 r_2 R^3} - \frac{15 r_2'}{4 r_2^2 R^6} + \frac{2025}{8 r_2^2 R^6} - \frac{7875 a_3}{2 R^7} - \frac{540 \sqrt{10}}{(-r_2)^{3/2} R^{15/2}} - \frac{1125 r_2'}{8 r_2^3 R^8} + O\left(\frac{1}{R^9}\right)].
\]

(21)
3. For f-wave resonance:

(a) \( m = 0, \)

\[
\kappa = \frac{\sqrt{63000}}{\sqrt{-r_3^2} R^{7/2}} \left[ 1 - \frac{a_0}{40R} + \frac{79a_0^2}{3200R^2} - \frac{3121a_0^3}{1250000R^3} + \frac{2a_0}{5R^5} + \frac{19731a_0^4}{81250000R^4} + \frac{57a_0}{100R^7} - \frac{3\sqrt{70} a_0^5}{2\sqrt{-r_3^2} R^{9/2}} + O\left( \frac{1}{R^9} \right) \right];
\]

(b) \( m = \pm 1, \)

\[
\kappa = \frac{\sqrt{47250}}{\sqrt{-r_3^2} R^{7/2}} \left[ 1 - \frac{3a_1}{5R^3} + \frac{15(147 - 10a_2r_3)}{2r_3 R^5} + \frac{81a_1^2}{50R^6} - \frac{7875r_3}{4r_3^3 R^7} + \frac{9a_1(-1407 + 50a_2r_3)}{2r_3 R^8} + O\left( \frac{1}{R^9} \right) \right];
\]

(c) \( m = \pm 2, \)

\[
\kappa = \frac{\sqrt{18900}}{\sqrt{-r_3^2} R^{7/2}} \left[ 1 + \frac{15(168 - 5a_2r_3)}{4r_3 R^5} - \frac{1575r_3^2}{2r_3^3 R^7} - \frac{4862025a_4}{4R^9} + \frac{225(155232 - 11760a_2r_3 + 95a_2^2r_3^2)}{32r_3 R^3} \right.
\]
\[
- \frac{366735600a_5}{R^{11}} + O\left( \frac{1}{R^{12}} \right);\]

(d) \( m = \pm 3, \)

\[
\kappa = \frac{\sqrt{3150}}{\sqrt{-r_3^2} R^{7/2}} \left[ 1 + \frac{315}{2r_3 R^5} - \frac{525r_3^2}{4r_3^3 R^7} - \frac{694575a_4}{2R^9} + \frac{628425}{8r_3^3 R^{10}} - \frac{137525850a_5}{R^{11}} + O\left( \frac{1}{R^{12}} \right) \right].
\]

From Eq. (17)-(25), we see that at the L-wave resonance, the leading order term in the expansion of \( \kappa \) is proportional to \( \frac{1}{\sqrt{R^{2L+1}}} \). The first order correction is due to the partial wave channels with orbital angular momentum quantum numbers equal to \( L \) or \( |m| \), while the higher order corrections are also influenced by other partial wave channels. By expanding \( \kappa \) to high powers of \( 1/R \), one will see the effects of all the effective range expansion parameters in all the channels that satisfy \( L \geq |m| \).

In general, the leading order terms for the binding energies at the L-wave resonance are

\[
E = \left\{ \begin{array}{ll}
\frac{k^2 \chi_0^2}{2m \ell^2}, & \text{if } L = 0, \\
\frac{k^2 \chi_0^2}{2m (-r_{L}^2 \chi_0^2)}, & \text{if } L \geq 1,
\end{array} \right.
\]

where \( \chi_0 \approx 0.567143 \) is the real solution to the equation

\[
\chi_0 = e^{-\chi_0}, \quad -L \leq m \leq L,
\]

and

\[
\chi_{Lm} = \frac{2 (2L + 1)! (2L - 1)! (2L)!}{(L - m)! (L + m)!}.
\]

To obtain Eq. (26) at \( L \geq 1 \), we used the following expansion at small \( x \):

\[
F_{LL}^m(x) = (-1)^{L-m+1} \frac{\chi_{Lm}}{2 x^{2L+1}} + O(x^{-2L}).
\]

When two heavy particles interact resonantly with a light particle by short-range potential, within the Born-Oppenheimer approximation they experience an effective potential equal to the binding energy \( E \) for the light particle. At an s-wave resonance, the \(-1/R^2\) dependence of the effective potential results in the appearance of three-body Efimov states \( 40 \). At higher partial wave resonances \( (L \geq 1) \), however, the three-body Efimov effect seems unlikely, because the Schrödinger equation for two heavy particles with effective potential \( \propto -1/R^{2L+1} \) has no scaling symmetry.

### IV. CORRECTIONS TO \( \kappa \) SLIGHTLY OFF RESONANCE

Since experimentally the scattering volume \( a_L \) cannot be tuned exactly to infinity, it would be nice to know the corrections to the expansions of \( \kappa \) in Eqs. (16)-(25) when \( a_L \) is large but finite. We use Eqs. (17)-(25) to calculate these corrections to the leading order in \( 1/a_L \). Our results are listed in Table I. In general, in the very vicinity of a resonance

\[
\kappa \approx \left\{ \begin{array}{ll}
\kappa_{\text{resonance}} + \frac{1}{\sqrt{-\chi_{Lm}^2 a_L}}, & \text{if } L = 0, \\
\kappa_{\text{resonance}} + \frac{1}{\sqrt{-\chi_{Lm}^2 a_L}}, & \text{if } L \geq 1.
\end{array} \right.
\]

To guarantee the applicability of the expansions in Eqs. (16)-(25), the above corrections must be small compared to the leading order term for \( \kappa \). This condition is met if \( |a_L|^{1/(2L+1)} \gg R \). Moreover, the effective range expansion Eq. (18) requires \( |kr_c| \ll 1 \), where \( r_c \) is the radius of the short-range potential between the atom and a scattering center. In many systems \( r_c \) can be characterized by the effective range \( r_L \), namely \( r_c \sim |r_L|^{1/(2L+1)} \). For such systems we obtain the domain of applicability...
calculate the binding energies versus

We use the above equation together with Eq. (4) to cal-

table I: The $O(1/\alpha L)$ corrections to $\kappa$ slightly away from resonance.

of the expansions in Eqs. (10) - (25):

$$|r_L|^{1/(2L+1)} \ll R \ll |a_L|^{1/(2L+1)}. \quad (30)$$

V. NUMERICAL RESULTS FOR THE BINDING ENERGIES NEAR A RESONANCE

When $R$ and $|a_L|^{1/(2L+1)}$ are both much larger than the radius $r_c$ of the potential, but $|a_L|^{1/(2L+1)}$ is comparable to $R$, we can no longer use series expansions to com-

pute the binding energies. Nevertheless, we can ignore the effects of the non-resonant channels (with $l \neq L$) in Eq. (11) to a good approximation. Keeping the first two terms in the effective range expansion for $k^{2L+1} \cot \delta_L(k)$, and noting that $k = i\kappa$, we get

$$1 + \frac{r_L}{\alpha L} - \kappa^2 \geq (1)^{L+1} \kappa^{2L+1} \left[ 1 + \sigma F_{L}(\kappa R) \right] = 0. \quad (31)$$

We use the above equation together with Eq. (4) to cal-

culate the binding energies versus $R$ for three fixed values of $a_L$ (large and positive, infinity, or large and negative) for each value of $L$. Our results are plotted in Fig. 1.

For the s-wave resonance ($L = 0$), we have neglected the effective range $r_0$; this is appropriate for broad s-wave Feshbach resonances [23, 24]. For p-wave and higher par-

tial wave resonances ($L \geq 1$), however, the effective range $r_L$ is important [24, 32-34, 37] and we have kept it in our calculations.

In Fig. 1 the power laws of Eq. (26) serve as asymptotes of the binding energies in the region $R \ll |a_L|^{1/(2L+1)}$.

If $a_L$ is large and negative or equal to infinity, we have a single shallow bound state for each orbital magnetic quantum number $m$ ranging from $L - 1$ to $L$. It is the “bonding state” discussed in Sec. II and its parity is $\sigma = (-1)^m$. If $a_L$ is large and negative, this bound state disappears when the distance between the two scattering centers exceeds a critical value,

$$R_c = \left( \frac{\chi L m}{2} |a_L| \right)^{1/(2L+1)}. \quad (32)$$

For the s-wave resonance, we recover the known result

$$R_c = |a_0| \quad [47].$$

For the p-wave or any higher partial wave resonance, Eq. (32) shows that the bound states with different values of $|m|$ disappear at different critical distances. The binding energy vanishes either quadratically or linearly when $R$ approaches $R_c$ from below, depending on $L$:

$$E \approx \begin{cases} \frac{k^2}{2M a_L} (|a_0| - R)^2, & L = 0, \\ \frac{k^2}{M R |a_L R|} (R - R_c), & L \geq 1. \end{cases} \quad (33)$$

If $a_L$ is large and positive, we have either one or two shallow bound states for each orbital magnetic quantum number $m$ ranging from $-L$ to $L$, depending on the distance $R$ between the two centers. For all $R$ there is a “bonding state” with parity $\sigma = (-1)^m$. If $R > R_c$ where $R_c$ is given by Eq. (32), there is an extra shallow state with parity $\sigma = (-1)^m+1$, namely the “anti-bonding” state discussed in Sec. II. When the two scattering centers are far apart ($R \to \infty$), the wave functions of both shallow states are localized near two separate centers, and their energies both exponentially approach the binding energy due to a single center:

$$E_1 = \begin{cases} \frac{k^2}{2M a_L} (R - a_0)^2, & L = 0, \\ \frac{k^2}{M |a_L R|} (R - R_c), & L \geq 1. \end{cases} \quad (34)$$

When $R$ approaches $R_c$ from above, the energy of the anti-bonding state vanishes linearly:

$$E \approx \begin{cases} \frac{k^2}{M a_L} (R - a_0), & L = 0, \\ \frac{k^2}{M |a_L R|} (R - R_c), & L \geq 1. \end{cases} \quad (35)$$

VI. A SIMPLE FORMULA FOR THE BINDING ENERGIES NEAR p-WAVE OR HIGHER PARTIAL WAVE RESONANCES

Near a $p$-wave or higher partial wave resonance, if $R, |a_L|^{1/(2L+1)} \gg |r_L|^{1/(1-2L)}$, the shallow bound states satisfy $\kappa R \ll 1$. Thus

$$(-1)^{L+1} \frac{\kappa^{2L+1}}{1 + \sigma F^m_{L}} (\kappa R) \approx \frac{\chi L m}{2} \sigma R^{-2L-1} + O(R^{-2L+1} \kappa^2), \quad L \geq 1, \quad (36)$$

where $\sigma \equiv \sigma /(-1)^m$ is the $z$-parity of the wave function; $\sigma$ equals 1 for bonding states and $-1$ for anti-bonding states [see Eq. (15)]. Further using the inequality $R^{-2L+1} \kappa^2 \ll |r_L| |\kappa|^2$ and Eq. (4), we can approximate Eq. (31) as

$$1 - \frac{r_L M E}{\hbar^2} + \frac{\chi L m}{2} \sigma R^{-2L-1} = 0 \quad \text{if } L \geq 1. \quad (37)$$

From the above equation we obtain a simple formula for the binding energy at $L \geq 1$:

$$\bar{E} = -\text{sign}(a_L) - \sigma \left( \frac{2L}{L - m} \right) P, \quad (38)$$
FIG. 1: (color online) The binding energy $E$ of a single atom interacting resonantly with two scattering centers separated by a large distance $R$, computed using Eq. (38) and Eq. (31). Solid lines are for scattering volumes $a_L = \pm \infty$. Dashed lines: $a_L$ is large and negative. Dot-dashed lines: $a_L$ is large and positive. The black, red, blue, and brown curves represent orbital magnetic quantum numbers $m = 0$, $m = \pm 1$, $m = \pm 2$, and $m = \pm 3$, respectively. The horizontal dotted line indicates the binding energy $E_1$ due to a single scattering center [see Eq. (34)]. We have chosen $|a_L|^{1/(2L+1)}/|r_L|^{1/(-2L+1)} = 50$ or $\infty$ in the plots for $L \geq 1$.

FIG. 2: (color online) The dimensionless energy $\tilde{E} = E/|E_1|$, where $E_1$ is defined in Eq. (34), versus the parameter $P = (2L + 1)!!/(2L - 1)!!|a_L|/R^{2L+1}$ near $p$, $d$, or $f$-wave resonance. Curves were computed by solving Eq. (34) numerically, but they have no visible differences from the predictions of the simple formula in Eq. (38). Curves with vertical intercept $-1$ are for $a_L > 0$ and those with (extrapolated) vertical intercept $+1$ are for $a_L < 0$. Curves with negative slopes are for bonding states and those with positive slopes are for anti-bonding states. Different colors indicate different values of $m$ as in Fig. 1; in each graph, the curves with steeper slopes have smaller values of $|m|$.
Equation \((38)\) illustrates the concept of universality in \(p\)-wave and higher partial wave Feshbach resonances. By normalizing the binding energy \(E\) by the energy due to a single scattering center with a positive scattering volume, and normalizing the distance by the scattering volume, we get the same set of universal relations between the dimensionless parameters \(E\) and \(P\) regardless of the atomic species or the Feshbach resonance concerned. When we plot \(E\) against \(P\), we shall find a set of straight lines with intercept \(-1\) for \(a_L < 0\) or \(+1\) for \(a_L > 0\); the absolute values of their slopes are given by the binomial coefficients \((2L - m)/(2L)\), with the lines for \(m = 0\) having the steepest slopes for a given \(L\). For example, for the \(d\)-wave resonance, the absolute values of these slopes have ratio \(1 : 4 : 6 : 4 : 1\).

In Fig. 2 we re-plot the energies obtained numerically from Eq. \((31)\). For the parameters we used [see the caption of Fig. 1], we find that the resultant curves have no visible differences from the predictions of Eq. \((38)\).

VII. EFFECTS OF THE VAN DER WAALS POTENTIAL

In the previous sections we assumed that the interaction potential between the atom and each scattering center strictly vanishes beyond a certain radius \(r_e\). If each scattering center is a pinned neutral atom and interacts with the free atom by a long range Van der Waals potential

\[
V(r) = -\frac{\hbar^2\beta_6^4}{2Mr^6}, \quad r \gg r_e, \tag{40}
\]

Eq. \((1)\) as well as the more general universal formula Eq. \((38)\) remain valid near \(p\)-wave and \(d\)-wave resonances \((L = 1, 2)\), but break down for \(L \geq 3\). The validity of Eqs. \((1)\) \((38)\) depends on the validity of the effective range expansion, Eq. \((13)\). For neutral atoms with a long range Van der Waals potential, the effective range expansion remains valid up to the first two terms on the right hand side of Eq. \((13)\) in the \(s\)-wave channel. \(48, 49, 50\) Near or at a \(p\)-wave resonance, Gao’s work \(44, 46, 50\) implies that the \(p\)-wave scattering length and effective range can also be defined \(44, 46, 50\). Ref. \(51\) discussed the conditions under which the effective range expansion remains valid.

Near a \(d\)-wave resonance, Gao’s work \(54, 52\) also implies that the first two terms of the effective range expansion for the \(d\)-wave phase shift are applicable within a certain window of collision energies. We have confirmed this by doing some simple perturbative expansions of the wave function (see Appendix A for details). In particular, we got

\[
\tan \delta_2(k) = \frac{\pi}{315}k^4 - \frac{\pi}{900\sqrt{2}\Gamma(5/4)^2} \left[ j + ck^2 + o(k^2^) \right], \tag{41}
\]

where \(k = \sqrt[4]{\beta_6}\), and the parameters \(j\) and \(c\) are determined by the short-range physics. Equation \((11)\) is consistent with Gao’s previous results \(50, 52, 53\). For safety we have verified Eq. \((11)\) numerically by solving the Schrödinger equation with the \(-C_6/r^6\) potential in three different cases: \(j = 0\), \(j = 1\), and \(j = 2\). Near \(d\)-wave resonance (so that \(j = 1\)) and at \(|j| < |k| < \frac{1}{\sqrt{2}}\), the term \(\frac{\pi}{315}k^4\) is negligible, and we reproduce two terms of the usual \(d\)-wave effective range expansion [Eq. \((13)\)] if we set

\[
a_2 = -\frac{\pi \beta_6^2}{900\sqrt{2}\Gamma(5/4)^2}, \quad r_2 = -\frac{1800\sqrt{2}\Gamma(5/4)^2c}{\pi \beta_6^2}. \tag{42}
\]

Thus, the first two terms in the effective range expansion [Eq. \((13)\)] remain applicable near \(s, p, d\)-wave Feshbach resonances. Using these formulas for the phase shifts and the approach developed in Sec. II we can derive Eq. \((1)\) as well as the more general universal formula Eq. \((38)\) in the presence of the Van der Waals potential for \(p\)-wave or \(d\)-wave resonances.

VIII. SUMMARY AND DISCUSSIONS

In summary, we have investigated the shallow bound states of a single atom interacting strongly with two scattering centers separated by a large distance \(R\). At \(s, p, d,\) or \(f\)-wave resonances, we have obtained systematic large-\(R\) expansions for the wave numbers of the bound states. Effects of non-resonant partial wave channels and the shape parameters in the effective range expansion enter as correction terms in these expansions. For a \(p\)-wave or higher partial wave resonance \((L \geq 1)\) the leading term for the binding energy behaves like \(-1/R^{2L+1}\) which, if combined with the Born-Oppenheimer approximation for two heavy and one light atoms, does not support three-body Efimov effect. Refs. \(34, 35\) contain more general discussions of the question of Efimov effect near higher partial wave resonances, without using the BO approximation.

Slightly off resonance we have found the \(O(1/a_L)\) corrections to the wave numbers for the bound states.

For large scattering volumes \(a_L\) and large distances \(R\) we have computed the energies of the shallow bound
states approximately, by ignoring the non-resonant partial wave scatterings and the shape parameters in the effective range expansion.

Finally, for \( p \)-wave and higher partial wave resonances, we have found a simple formula for the binding energies, Eq. (38), assuming that \( R \) and \( |a_L|^{1/(2L+1)} \) are both large but may be comparable to each other. Experimental confirmation of this formula will demonstrate the notion of universality in higher partial wave resonances.

Although we mainly considered short-range interactions between the scattering centers and the atom, we have found that a long range Van der Waals potential will not undermine our central results, such as Eqs. (11) and (A1), near \( p \) and \( d \)-wave resonances \( (L = 1, 2) \).

It is worthwhile to point out a technical limitation of our present work. We have not taken into account the orbital magnetic quantum number \( l_m \), etc in our formulas by \( a_{lm} \) and \( r_{lm} \) etc. Moreover, if the higher partial wave resonance between the atom and each scattering center is physically a confinement-induced resonance due to an underlying \( s \)-wave Feshbach resonance, one can have a nearly isotropic effective interaction – provided that a spherically symmetric trap is used to confine each pinned atom which, in turn, serves as a scattering center.

To realize the scenario of one atom interacting with two fixed centers, it is not necessary to use two atomic species with a large ratio of bare masses. If two atoms of species A are pinned at two lattice sites of an optical lattice, but an atom of species B is not attracted or repelled by the lattice, we can treat atoms A as infinitely heavy scattering centers for atom B.

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\section*{Note Added}

Near completion of this work an analogous study focused on \( p \)-wave resonance appeared online [54].

\section*{Appendix A: \( d \)-wave phase shift in the presence of a Van der Waals potential}

In this appendix we derive a formula for the \( d \)-wave scattering phase shift \( \delta_2 \) for a potential that behaves as

\begin{equation}
\text{Eq. (40).}
\end{equation}

At \( r \gg r_c \) the \( d \)-wave radial Schrödinger equation is

\begin{equation}
-u''(r) + \left( \frac{6}{r^2} - \frac{\beta_2}{r^4} \right) u(r) = k^2 u(r),
\end{equation}

where \( u(r) \equiv r\psi(r) \). In the following we set the Van der Waals length \( \beta_2 = 1 \) for convenience.

Assuming that \( k \ll 1 \), we solve Eq. (A1) in two regions:

- **Region I:** \( r \ll 1/k \);
- **Region II:** \( r \gg 1 \).

Then, we require the two solutions to be the same in the intermediate region, \( 1 \ll r \ll 1/k \). From this condition we obtain an approximate formula for the \( d \)-wave phase shift \( \delta_2 \).

In the region \( r \ll 1/k \), we can treat the term \( k^2 u(r) \) in Eq. (A1) as a perturbation, and expand \( u(r) \) in powers of \( k^2 \):

\begin{equation}
u(r) = f(r) + j\tilde{f}(r) + k^2 [g(r) + j\tilde{g}(r) + cf(r)] + O(k^4)
\end{equation}

under a suitable normalization. Here

\begin{equation}f(r) = \sqrt{r} J_{5/4}\left(\frac{1}{2r^2}\right)\end{equation}

and

\begin{equation}\tilde{f}(r) = \sqrt{r} J_{-5/4}\left(\frac{1}{2r^2}\right)\end{equation}

are two independent solutions of the zero-energy radial Schrödinger equation

\begin{equation}\hat{H}f(r) = 0,\end{equation}

where \( \hat{H} \equiv -\frac{d^2}{dr^2} + \frac{\beta_2}{r^4} - \frac{1}{r^2} \), and \( J_n(x) \) is the Bessel function. The functions \( g(r), \tilde{g}(r) \) are the solutions to the following equations

\begin{equation}\hat{H}g(r) = f(r),\end{equation}

\begin{equation}\hat{H}\tilde{g}(r) = \tilde{f}(r),\end{equation}

subject to the conditions Eq. (A10) and Eq. (A11) below. At large \( r \), the functions \( f(r), \tilde{f}(r), g(r), \tilde{g}(r) \) have the following asymptotic expansions:

\begin{equation}f(r) = \frac{1}{5\sqrt{2}\Gamma(5/4)} \frac{1}{r^2} + O(r^{-6}),\end{equation}

\begin{equation}\tilde{f}(r) = \frac{4\sqrt{2}}{\Gamma(-1/4)} r^3 + \frac{\sqrt{2}}{\Gamma(-1/4)r} + O(r^{-5}),\end{equation}

\begin{equation}g(r) = \frac{1}{30\sqrt{2}\Gamma(5/4)} + O(r^{-4}),\end{equation}

\begin{equation}\tilde{g}(r) = \frac{2\sqrt{2}}{7\Gamma(-1/4)} r^5 + \frac{5}{21\sqrt{2}\Gamma(-1/4)r} + O(r^{-3}).\end{equation}
The constants $j$ and $c$ are determined by the short-range physics. At resonance, $j = 0$ and the zero-energy solution for $u(r)$ decays like $r^{-2}$ at large $r$, consistent with the picture of a bound state at threshold. Slightly away from $d$-wave resonance $j$ is close to zero and may take either sign.

In the region $r \gg 1$, we can treat the term $\frac{\delta^2}{r^2} u(r)$ in Eq. (A1) as a perturbation, and obtain another expansion for $u(r)$:

$$u(r) = A(k) \left\{ \sum_{n=0}^{\infty} k^{4n} V_n(kr) - \left[ \tan \delta_2(k) \right] \sum_{n=0}^{\infty} k^{4n} W_n(kr) \right\}, \quad (A12)$$

where $A(k)$ is a normalization factor depending on $k$ only,

$$V_0(\xi) = \xi j_2(\xi), \quad W_0(\xi) = \xi n_2(\xi), \quad (A13)$$

$j_2(\xi)$ and $n_2(\xi)$ are the spherical Bessel functions, and $V_2(\xi)$ and $W_2(\xi)$ are defined by the equations

$$-V_n''(\xi) + \left( \frac{6}{\xi^2} - 1 \right) V_n(\xi) = \frac{1}{\xi^6} V_{n-1}(\xi), \quad (A14)$$

$$-W_n''(\xi) + \left( \frac{6}{\xi^2} - 1 \right) W_n(\xi) = \frac{1}{\xi^6} W_{n-1}(\xi), \quad (A15)$$

subject to the condition that $V_n(\xi)$ and $W_n(\xi)$ are oscillating decaying functions at $\xi \to \infty$ for $n \geq 1$.

When $\xi \to 0^+$ we have

$$V_0(\xi) = \frac{\xi^3}{15} + O(\xi^2), \quad (A16)$$

$$W_0(\xi) = -\frac{3}{\xi^2} \frac{1}{2} - \frac{\xi^2}{8} + O(\xi^4), \quad (A17)$$

$$V_1(\xi) = -\frac{\pi}{105 \xi^2} + O\left( \frac{1}{\xi^2} \right), \quad (A18)$$

$$W_1(\xi) = \frac{1}{12 \xi^2} + O\left( \frac{1}{\xi^4} \right). \quad (A19)$$

In the intermediate region, $1 \ll r \ll 1/k$, we obtain from Eq. (A2)

$$u(r) \propto \left[ j + ck^2 + O(k^4) \right] r^3 - \frac{\pi}{20 \sqrt{21} (5/4)^2} \frac{1}{r^2} \frac{1}{15} + O(k^6) + O(k^7 \tan \delta_2) \right] r^3$$

$$+ \left\{ -\frac{\pi k^2}{105} + o(k^5) + \left[ \frac{3}{k^2} + o(k) \right] \tan \delta_2 \right\} r^{-2} + \text{other powers of } r. \quad (A21)$$

Note that the “other powers of $r$” include terms of the order $r^n \ln r^m$ for integers $n$ and $m$, with $n \neq -2, 3$. Comparing the above two formulas for $u(r)$ in the intermediate region, we get the expression Eq. (11) for the phase shift $\delta_2$.

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