Universal two-body spectra of ultracold harmonically trapped atoms in two and three dimensions

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Abstract
We consider the spectrum of two ultracold harmonically trapped atoms interacting via short-range interactions. The Green function approach is used to unify the two- and three-dimensional cases. We derive criteria for the universality of the spectrum, i.e. its independence of the details of the short-range interaction. The results in three dimensions are exemplified for narrow s-wave Feshbach resonances and we show how effective range corrections can modify the rearrangement of the level structure. However, this requires extremely narrow resonances or very tight traps that are not currently experimentally available. In the two-dimensional case, we discuss the p-wave channel in detail and demonstrate how the non-universality of the spectrum arises within the Green function approach. We then show that the spectrum is not particularly sensitive to the short-distance details in the case when the two-body interaction has a bound state.

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(Some figures may appear in colour only in the online journal)

1. Introduction

In an age of rapidly increasing computational power, exact methods and benchmark solutions continue to have tremendous importance as a means of gauging numerical calculations and provide invaluable analytical insights [1]. Ultracold atomic gases have emerged as a field with great potential as a laboratory benchmark for many fields of physics. The extreme control exercised over the systems in terms of trapping geometry and inter-atomic interactions allow experimenters to prepare samples that simulate the intricacies of many different models that are applied in other fields of physics and the term ‘quantum simulator’ is often applied [2]. The clean conditions provide hope of understanding some of the paradigmatic models such as the Hubbard model that are used frequently in the study of materials and other condensed-matter systems.
In the case of cold atoms, the interactions are typically short-ranged and the samples have to be in an external confinement, most often provided by a magnetic or optical potential. In the case of a harmonic oscillator trapping potential, it turns out that the problem of two atoms interacting through a short-range potential can be exactly solved as demonstrated by Busch et al [3]. The authors of [3] approximated the two-body interaction potential by a zero-range pseudopotential introduced long ago by Hellmann [4] and Fermi [5]. The predictions of this exact model were subsequently tested experimentally in an optical lattice and found to be a very accurate description of the two-atom system [6].

The pseudopotential approach has become somewhat of a paradigm itself in cold atoms. Its success can largely be attributed to a separation of scales; the two-body collision energy is small at the low temperatures that one usually aims for, and the density of the system is also much lower than typical matter densities. One can then model the interaction using only a few low-energy parameters such as the scattering length $a$ and effective range $r_e$ [7]. The true range of the potential, given by the van der Waals length for neutral atoms, is much smaller than the interparticle spacing. The parameters $a$ and $r_e$ therefore characterize the system, and since these are independent of the shape of the two-body potential, one refers to this as a universal regime, i.e. when $|a|, n^{-1/3} \gg r_0$ with $n$ being the density. A really nice feature of the cold atomic gas system is the tunability of the interaction parameters through Feshbach resonances [8], which allows one to explore the full region of parameter space, including the interesting unitarity limit, where $1/|a| \to 0$.

In the case of a trapped system with harmonic oscillator length $b$, a fundamental question concerns the binding energy of an $N$-body system in the universal regime when we also require that $r_0 \ll b$. For equal mass particles, this has been studied numerically using a host of different methods [9]. Interestingly, for $a \to \infty$, the three-body problem in a trap can be exactly solved [10]. In the same spirit, exactly solvable models in a harmonic approximation approach have been proposed [11]. Very recently, experiments in the so-called microtraps have demonstrated that few-body systems can in fact be produced with cold atoms, and universality and shell structure can be explored [12]. The general framework of effective field theory is very suitable for problems with separation of scales, and it has been applied successfully to the three-body problem in cold atoms [13]. Recently, there has been a lot of interest in applying these techniques within an oscillator basis [14, 15] to address few-body Fermi systems in cold atoms and in nuclei within the no-core shell-model approach [16]. Similar methods have also been used to study few-body bosonic systems in traps (see [17] and [18] for details and references).

The model of Busch et al is the basic foundation upon which many of the developments discussed above reside. Here, we take a fresh look at the model from a Green function point of view [21, 20, 19]. This is done within a two-channel formalism. We consider the general angular momentum $l$-wave case and derive the expression for the eigenspectrum in three dimensions as a function of the scattering phase shift. For $l \geq 2$, there are obstructing terms that imply a dependence on the short-range two-body potential, i.e. the spectrum is non-universal. A criterion for the applicability of the universal formula is subsequently derived.

As an example, we consider a two-channel model for narrow Feshbach resonances and show that interesting spectral changes occur when including the effective range term. This can be interpreted in terms of the Zeldovich rearrangement effect [22], which occurs in systems with a long-range attractive potential and a short-range two-body attraction that dominates at small distance (some recent discussion of the effect can be found in [23, 24]). The observation of these effects in experiments require, however, extremely tight trapping potentials or extremely narrow Feshbach resonances, both of which are beyond the current experimental capabilities.
Two-dimensional setups are currently of great interest in the cold atom community and a number of impressive experimental results have been reported recently [25]. In the second part of the paper, we consider a two-dimensional geometry and derive the eigenspectrum within the Green function approach. We find that for the angular momentum \( m \geq 1 \), there are non-universal terms, i.e. a spectrum that depends on the short-range details of the two-body potential. Emphasis is put on the p-wave case \( m = 1 \), where we find a closed formula for the spectrum in terms of the low-energy parameters of the interaction. To obtain the eigenspectrum, we use a generic form of the p-wave phase shift in two dimensions, which is similar to that obtained in hard-sphere or square-well potential models. The p-wave spectrum in the case where the interaction allows a two-body bound state is very similar to that of s-waves. The shape of the p-wave spectrum is almost universal, depending only slightly on the exact potential model used.

2. Basic two-channel formalism

The physics around Feshbach resonances [8] is most naturally described by models that explicitly take the open (scattering) channel and the closed (molecular) channel into account [26, 8]. Here, we consider such a model within the Green function approach [21]. The setup has a dressed state with open- and closed-channel wavefunctions, \( \Psi_1(r) \) and \( \beta \phi(r) \), respectively, where \( \beta \) is the amplitude of the closed channel and the normalization is \( |\beta|^2 + \int dr |\Psi_1(r)|^2 = 1 \) since we assume that \( \phi \) is normalized. The Hilbert space of the closed channel is therefore one dimensional for simplicity. Note that \( \phi(r) \) has an angular momentum \( l \) and projection \( m_l \).

The wave equations are

\[
D_{\text{trap}} \Psi(r) + W(r) \beta \phi(r) = E \Psi(r),
\]

\[
W(r) \Psi(r) + E_{\text{mol}} \beta \phi(r) = E \beta \phi(r),
\]

where the operator is \( D_{\text{trap}} = D_{\text{free}} + V(r) \). Here, \( V(r) \) is the trapping potential that we assume to be an isotropic harmonic oscillator with the trap length \( b = \sqrt{\hbar/\mu \omega} \), where \( \omega \) is the oscillator frequency and \( \mu \) is the reduced mass, i.e. \( V(r) = \frac{1}{2} \mu \omega^2 r^2 \). The free-particle operator has the standard form \( D_{\text{free}} = -\hbar^2 \nabla^2 / 2\mu \). The energy of the closed channel molecule is denoted \( E_{\text{mol}} \) and the coupling between the channels is parametrized by the real function \( W(r) \). We assume that the range of \( W(r) \) is much smaller than \( b \).

3. Three dimensions

The 3D Green function \( G_E(r, r') \) is defined by

\[
[D_{\text{trap}} - E] G_E(r, r') = \frac{2\pi \hbar^2}{\mu} \delta(r - r').
\]

If we define

\[
F = E - E_{\text{mol}} + \frac{\mu}{2\pi \hbar^2} \int dr \, dr' \phi^*(r) G_E(r, r') \phi'(r'),
\]

where \( \phi(r) = W(r) \phi(r) \), then upon substitution of equation (3) into equations (1) and (2) we obtain \( F = 0 \). In momentum space, we have \( \phi(k) = \sqrt{4\pi} \sqrt{k^2} Y_{lm}(k) \alpha_{lm} \), which defines the coupling constant [19]

\[
\alpha_{lm} = \sqrt{4\pi} k^{-1} \int dr \, \phi(r) j_l(kr) Y_{lm}^*(r).
\]
In order to relate the spectrum in the trap to the free-particle scattering properties, we have to calculate the scattering amplitude. Therefore, we consider the scattering problem

\[ \Psi(r) = e^{ikr} - \frac{\mu}{2\pi\hbar^2} \beta \int \frac{dr'}{F_0} \hat{\phi}(r') G^0_E(r, r'), \]

where \( G^0_E(r, r') \) is the free-particle Green function and \( E = \hbar^2 k^2 / 2\mu \) is the scattering energy (see appendix A). Solving for \( \beta \) in equation (2) and inserting into the scattering solution in equation (6), we find

\[ \Psi(r) = e^{ikr} - \frac{\mu}{2\pi\hbar^2} \hat{\phi}^*(k) \int \frac{dr'}{F_0} e^{-ikr'} G^0_E(r, r'), \]

where \( F_0 \) is defined analogous to \( F \) above but with the free Green function \( G^0_E(r, r') \). The solution of equation (3) for out-going wave boundary conditions when the trap is absent has the asymptotic behavior

\[ G^0_E(r, r') = \frac{e^{ikr}}{|r - r'|} \rightarrow \frac{e^{-ikr}}{r} \quad \text{for} \quad r \rightarrow \infty, \]

where \( k' \) is the final momentum that fulfills \( |k| = |k'| \). Using the fact that

\[ \hat{\phi}^*(k) = \int dr e^{-ikr} \hat{\phi}(r), \]

we finally obtain

\[ f_k(k') = -\frac{\mu}{2\pi\hbar^2} \hat{\phi}^*(k) \hat{\phi}(k'). \]

Through partial wave decomposition \( f_k(k') = 4\pi \sum_{lm} f_{lm}(k) Y^*_lm(k) Y_{lm}(k') \), we obtain

\[ \frac{|\alpha_{lm}|^2 k^2}{f_{lm}(k)} = \frac{2\pi \hbar^2}{\mu} (E_{\text{mol}} - E) - \int dr dr' \hat{\phi}^*(r) G^0_E(r, r') \hat{\phi}(r'). \]

Since both \( G^0_E(r, r') \) and \( G_E(r, r') \) are singular at \( r = r' \), we have to regularize by isolating the finite part through \( G^0_E(r, r') = G_E(r, r') - G^0_E(r, r') \). We find

\[ \frac{|\alpha_{lm}|^2 k^2}{f_{lm}(k)} = \int dr dr' \hat{\phi}^*(r) G^0_E(r, r') \hat{\phi}(r'), \]

where \( G^0_E(r, r') \) satisfies

\[ (D_{\text{trap}} - E) G^0_E(r, r') = -V(r) G^0_E(r, r'). \]

By symmetry, we only need to consider \( r > r' \), and we therefore write

\[ G^0_E(r, r') = g_t(r, r') j_0(kr') Y^*_lm(\hat{r}) Y_{lm}(\hat{r'}), \quad r > r'. \]

The solution for \( g_t(r, r') \) can easily obtained by noting that a particular solution to equation (13) is \(-G^0_E(r, r') \) [19]. Adding the homogenous solution gives

\[ g_t(r, r') = e^{-\frac{\mu}{2\pi} \left( A(r') \left( \frac{r}{b} \right)^l M(-\mu_1, l + 3/2; r^2/b^2) + B(r') \left( \frac{b}{r} \right)^{l+1} M(-\mu_2, 1/2 - l; r^2/b^2) \right) - 4\pi i k h_{1/2}^{(1)}(kr)}, \]

with \( \mu_1 = \frac{E}{2\mu} - 1/2 - 3/4 \) and \( \mu_2 = \frac{E}{2\mu} + 1/2 - 1/4 \). Here, \( M(a, b; x) \) is the confluent hypergeometric function and \( h_{1/2}^{(1)}(x) \) is the spherical Hankel function of the first kind. Demanding that \( G^0_E(r, r') \) vanishes as \( r \rightarrow \infty \) yields

\[ A(r') = -\frac{\Gamma(1/2 - l) \Gamma(-\mu_1)}{\Gamma(l + 3/2) \Gamma(-\mu_2)} B(r'). \]
Furthermore, by demanding that \( G_0^p(r, r') \) be regular as \( r, r' \to 0 \) (while maintaining the condition \( r > r' \)), we demand that

\[
\lim_{r' \to 0} B(r') = \frac{\Gamma(l + 1/2)}{b} \frac{2^{l+2} \sqrt{\pi}}{(kb)^l}.
\]

(17)

g_{l}(r, r') can now be determined for small \( r \). For \( r \to 0 \) and \( l \leq 2 \)

\[
g(r, r') \approx \frac{4\pi (kr)^l}{(2l + 1)!k^{2l}} \left[ \frac{(2l + 1)!!A(r')k^l}{4\pi b^l} - i^{k^{2l+1}} \right],
\]

(18)

where the leading term \( j_l(kr) \) for \( kr \ll 1 \) has been isolated to resemble the structure of equation (5). The imaginary part of equation (18) comes directly from \( \text{Im}[h^{(1)}_l(kr)] \). For \( l > 2 \), there are additional terms at order \( r^a \) with \( a < l \). Inserting the solution into equation (12) and assuming that \( \phi \) is short-ranged, we find

\[
f_{lm}(k) = \left[ \frac{(2l + 1)!!A(0)k^l}{4\pi b^l} - i^{k^{2l+1}} \right]^{-1},
\]

(19)

where \( a_{lm} \) cancels which was the object of the regularization procedure. Note that this does not depend on \( m \) due to the isotropy of the trap potential. Using equations (16) and (17), we finally have

\[
f_{lm}(k) = \left[ \frac{(-1)^{l+1} 2^{2l+1}}{b^{2l+1}} \frac{\Gamma(-\mu_1)}{\Gamma(-\mu_2)} - i^{k^{2l+1}} \right]^{-1}.
\]

(20)

This has to be related to the scattering amplitude in terms of the l-wave phase shift, \( b_l(k) \), which is

\[
f_{lm}(k) = \frac{k^{2l}}{k^{2l+1} \cot \delta(k) - i^{k^{2l+1}}}. \tag{21}
\]

Matching with the solution above, we obtain

\[
\frac{\Gamma \left( \frac{3}{2} + \frac{l}{2} - \frac{E}{2mb} \right)}{\Gamma \left( \frac{1}{4} - \frac{l}{2} - \frac{E}{2mb} \right)} = \frac{(-1)^{l+1} (kb)^{3l+1} \cot \delta(k)}{2^{2l+1}},
\]

(22)

which recovers previous results [3, 19, 27]. Furthermore, the expression in equation (22) shows how to include higher order terms from effective-range expansions.

The result in equation (19) holds for short-ranged \( \phi \) and for \( l < 2 \). There are generally \( r^a \) terms obstructing the simple formula derived above for \( l \geq 2 \). These have order from \( a = 3 - l \) to \( a = l - 1 \) in steps of 2 up to the leading \( A(0) \) term of order \( l \). For instance, the \( l = 2 \) case has a term proportional to \( r \), the \( l = 3 \) case has a constant and an \( r^2 \) term and so forth. This can be seen by considering the series expansion of \( h^{(1)}_l(x) \). Since we demand that \( \phi \) is very short-ranged, we assume \( r/b \ll 1 \). In general, the most important term near \( r = 0 \) will be \( r^{3-l} \) for \( l \geq 2 \); thus, it diverges for \( l > 3 \) that must be compensated by the behavior of \( \phi \). A sensible criterion for this to happen is that \( A(0) \) should dominate over the most divergent obstructing term. For general \( l \geq 2 \), this gives us the inequality

\[
\left| A(0) \right|^{l} < \frac{2^{l} \sqrt{\pi} \Gamma(l + 1/2)}{(2l - 3)(kb)^l} \left( \frac{r}{b} \right)^{3-l}.
\]

(23)

\( r \) is assumed to be of short-range and \( \phi(r) \) is an l-wave wavefunction. Thus, there will be some intermediate region around \( r = r_0 \), where \( \phi \) has its weight. We want the condition to be satisfied at this distance. Inserting \( A(0) \) and using equation (22), we arrive at

\[
\left( \frac{r_0}{b} \right)^{2l-3} \gg \frac{2l + 1}{2l - 3} \left( \frac{[2l(2l - 1)!]^l}{4} \right) \left| \tan \delta_l(k) \right| (kb)^{2l+1},
\]

(24)
which agrees with [27] for \( l = 2 \). The distance \( r_0 \) is essentially the same as the matching
distance of [28] and [27]. We still require \( r_0/b \ll 1 \), so when the right-hand side blows up, the
universal formula breaks down and the details of the two-body interaction become important.

For concreteness, let us consider a model for the coupling between the channels where
\( W(r) = W_0 e^{-r/\mu} \), with \( \alpha_0 \) being the Bohr radius [29]. Assuming that \( \phi(r) \propto r^l \), the
maximum of \( \phi \) is at \( r_0 = \alpha_0 \). The left-hand side of equation (24) is therefore very small as
\( b \sim 1 \mu \text{m} \) for typical traps. The factors depending on \( l \) on the right-hand side are increasing
but only gradually. Using the lowest order in the effective-range expansion, the criterion is
\( (a_l/b)^{2 l+1} \ll 1 \), where \( a_l \) is the \( l \)-wave scattering length (whenever it is well defined). Thus,
we conclude that the formula works only away from resonance.

3.1. 3D Feshbach model

The formula in equation (22) has been discussed by a number of authors for s-waves
[3, 30, 28], p-waves [20, 19] and d-waves [27]. In the context of Feshbach resonances,
most studies have assumed that the effective range can be neglected, which is true for wide
resonances [8]. To complement this, we considered here the opposite limit of very narrow
resonances where the effective range is large. This is interesting in cold atomic gases with two
or more different species of atoms, which typically have narrow resonances. In particular, at
the point where the scattering length tends to zero, we expect the corrections from higher order
terms to become important [31]. The universal behavior of one-channel models is described
through one parameter, i.e. the scattering length. As a function of applied external magnetic
field we parametrize the l-wave field-dependent scattering length \( a_l(B) \) in the following way:

\[
d^l(B)^{2l+1} = (a_{bg}^l)^{2l+1} \left[1 - \frac{\Delta B}{B - B_0}\right],
\]

where \( a_{bg}^l \) is the background scattering length away from the resonance located at \( B = B_0 \) with
width \( \Delta B \). Since we are interested in going beyond the one parameter description, we use a
two-channel model of a Feshbach resonance [32] with the corresponding open–open channel
s-wave \( T \)-matrix

\[
T_{oo}^s = \frac{2\pi \hbar^2 \alpha_0}{\mu} \left(1 + \frac{\Delta \mu \Delta B}{2 \hbar^2 \omega (E - \Delta \mu (B - B_0))}\right)^{-1} + i a_{bg}^l \frac{k}{\mu},
\]

where \( \Delta \mu \) is the difference in the magnetic moment of the open and closed channels.
Combining this with equation (20), we obtain

\[
\frac{b}{a_{bg}^l} \left(1 + \frac{\Delta \mu \Delta B}{E - \Delta \mu (B - B_0)}\right)^{-1} = \sqrt{2} \frac{\Gamma \left(\frac{1}{2} - \frac{E}{2 \omega a_{bg}^l}\right)}{\Gamma \left(\frac{1}{2} + \frac{E}{2 \omega a_{bg}^l}\right)},
\]

Introducing the background effective range \( r_{e0}^l = -\hbar^2 / (\Delta \mu \Delta B a_{bg}^l) \), and the useful quantities
\( x = (B - B_0) / \Delta B \) and \( f(E) = \sqrt{2} \pi \left(\frac{3}{4} - \frac{E}{2 \omega a_{bg}^l}\right) / \Gamma \left(\frac{1}{4} - \frac{E}{2 \omega a_{bg}^l}\right) \), we have

\[
\left(1 + \frac{1}{2a_{bg}^l \omega^{(l)}} E \frac{b}{b} \right)^{-1} = \frac{a_{bg}^l}{b} f(E).
\]

We note that since \( a_{bg}^l \Delta \mu \Delta B > 0 \) for all resonances with any \( l \) [8], we have \( r_{e0}^l < 0 \) always.
Isolating \( x \) yields

\[
x = \frac{1}{2} \frac{a_{bg}^l}{b} \frac{r_{e0}^l}{b} E - \frac{a_{bg}^l f(E)}{2 \frac{b}{b} \frac{b}{b} \hbar \omega - \frac{a_{bg}^l}{b} f(E)},
\]

In the case of a wide resonance or a large trap \( |r_{e0}^l|/b \rightarrow 0 \), we recover \( \frac{b}{b} f(E) \rightarrow f(E) \).
Figure 1. 3D s-wave spectrum with $a_s^*/b = 0.01$ and (a) $r_{\text{eq}}/b = 0.1$, (b) $r_{\text{eq}}/b = 1$, (c) $r_{\text{eq}}/b = 10$ and (d) $r_{\text{eq}}/b = 100$. The solid (black) lines denote the full solutions, while the dashed (red) lines are for $r_{\text{eq}} = 0$. The dot–dashed (blue) horizontal lines indicate the non-interacting level structure (visible at the top left corner of (a) and (b)), while the dotted (blue) vertical lines are asymptotes $\hbar \omega$ above (or below) the non-interacting levels.

There is one caveat that has to be addressed before we proceed to study the effective range corrections to the two-body spectrum. This is related to the limit when the scattering length becomes very small. Here, it is not necessarily clear that the properties of the spectrum will be universal in the sense that higher order parameters from the effective range expansion (beyond $a$ and $r_e$) can be neglected. This issue has been discussed in the context of effective field theory in [33].

The details of Feshbach resonances when the scattering length tends to zero have been considered for both trapped bosons and fermions in [31]. There it was found that the effective interaction is quadratic in the relative momentum at lowest order, since the usual constant piece proportional to $a_s^*$ vanishes. The coefficient depends on the background parameters of the resonance through the combination $(a_s^* b_{\text{bg}})^2 r_{\text{eq}}$. The studies in [31] demonstrated that no anomalous behavior is seen when approaching the zero-crossing of the Feshbach resonance.

Of course, if this quantity happens to be very small, even higher order terms in the effective-range expansion must be taken into account. Here, we are assuming that $|a_s^* b_{\text{bg}}| \gg r_{\text{vdW}}$ is much larger than the true range of the potential, given by the van der Waals length $r_{\text{vdW}}$. Likewise, for the narrow resonances, here we are interested in $|r_{\text{eq}}| \gg r_{\text{vdW}}$. It is in this regime that we expect the behavior to be universal, since this implies that low-energy scattering still dominates the two-body collisional dynamics. The smallest values used below are $a_s^*/b = 0.01$. For a typical trap with $b \sim 1 \mu m$, this is larger than $r_{\text{vdW}}$ for most atoms used in cold gas experiments.

In figures 1–3, the two-body spectrum in the trap is plotted for s-wave interactions and various values of the background parameters of the resonance, i.e. $a_s^* b_{\text{bg}}$ and $r_{\text{eq}}^*$, as a
function of $a''(B)/a_{bg}''$. We plot both the full solution and the standard case with $r_{c0} = 0$ for comparison. In figure 1, $a_{bg}'/b = 0.01$ that is very small. This means that the spectrum is almost equal to the non-interacting case when $r_{c0}'$ is also small. Note that the molecular state has energy proportional to $-(a_{bg}')^{-2}$ so its energy is below the range of the figure in the case of $r_{c0}' = 0$. In figures 1(c) and (d), the situation changes and a molecular state can be seen. One also clearly see the Zeldovich rearrangement effect [22, 23] of the levels on the right of figure 1(c) and middle of figure 1(d). The connection between the Busch model and this effect in the $r_{c0}' = 0$ case was discussed recently by Farrell et al [24]. However, the $a''(B)$ value of the rearrangement can now depend on the level since we have the term linear in $E$ in equation (29).

In contrast, for $r_{c0}' = 0$, the rearrangement occurs at $a''(B) = 0$.

In figures 2 and 3, we exhibit the spectrum for larger values of $a_{bg}'/b$, which means that the molecular state is now seen even for small $r_{c0}'$. From these figures, it is also clear that for large $r_{c0}'/b$ the rearrangement happens when $a''(B) = a_{bg}''$. This can again be understood from equation (29) since $x \to \infty$ when $a''(B) \to a_{bg}''$ and which implies $1 = a_{bg}'' f(E)/b$. The presence of the linear $E$ term for $r_{c0}' > 0$ gives distortion to this simple picture and enriches the rearrangement effect. Note that in figure 3(a), the lowest state shown is in fact not the molecular state but the first excited state. As $r_{c0}'$ increases, the molecular state is pulled up in energy as shown in figure 3(b). Also, figure 3(d) demonstrates that for very large values of $r_{c0}'$, the region where the levels rearrange can become very small, yielding almost abrupt jumps in the spectrum.

To access the spectra above experimentally will require large values of $a_{bg}'/b$ and $r_{c0}'/b$. For typical traps with $b$ of order $\mu$m, this seems inaccessible. However, a single site of an
optical lattice could have a much smaller \( b \) and has been used before to probe the two-body spectrum [6]. Assuming that one could make large reduction in \( b \), we still require Feshbach resonances with large background parameters. Atoms like \(^{23}\text{Na}\) or \(^{87}\text{Rb}\) do in fact have the known Feshbach resonances that are extremely narrow [8] and will give \( r_{e0} \) of order \( \mu \text{m} \). Resonances between two different mass atoms also tend to be narrow in general so mixtures are an option. However, narrow resonances require the ability to tune the magnetic field extremely precisely. The level of tunability required here is probably beyond any current experiment but will perhaps be available in next-generation experimental setups.

4. Two dimensions

The two-dimensional case is similar but contains the peculiarities of 2D scattering [34]. The free 2D Green function with an out-going boundary condition is

\[
G^0_E(\mathbf{r}, \mathbf{r}') = -i \frac{\mu}{2\hbar^2} H^{(1)}_0(k|\mathbf{r} - \mathbf{r}'|),
\]

where \( H^{(1)}_m(x) \) is the \( m \)th-order Hankel function of the first kind. We use the partial wave decomposition of Green’s function (see appendix A)

\[
G^0_E(\mathbf{r}, \mathbf{r}') = i\pi \sum_{m=-\infty}^{\infty} J_m(kr') H^{(1)}_m(kr),
\]
for \( r > r' \). \( J_m(x) \) is the Bessel function of order \( m \). The coupling constant \( \alpha_m \) has to be modified slightly to fit the 2D geometry. We define

\[
\alpha_m = \frac{\sqrt{\pi}}{k|m|} \int dr J_{|m|}(kr) e^{im\theta} \tilde{\phi}(r),
\]

where \( \tilde{\phi}(r) = \phi(r)W(r) \) just like in the 3D case above and \( \theta_r \) is the angle of the 2D vector \( r \).

For a wavefunction with the angular momentum \( m \), the Fourier transform becomes

\[
\tilde{\phi}(k) = \frac{1}{\sqrt{\pi}} \sum_{m=-\infty}^{\infty} r^m k^{|m|} \alpha_m e^{im\theta_0}.
\]

The finite part of the 2D Green function has to fulfill

\[
\frac{|\alpha_m|^2 k^{2|m|}}{f_m(k)} = \int dr dr' \tilde{\phi}^*(r) G^R_m(r, r') \tilde{\phi}(r'),
\]

where \( G^R_m(r, r') \) satisfies once again equation (13) and the scattering amplitude \( f_m(k) \) is connected to the scattering phase shift \( \delta_m(k) \) through [34]

\[
f_m(k) = \frac{k^{2|m|}}{\cot \delta_m(k) - ik^{2|m|}}.
\]

This can be solved similarly to the 3D case by assuming that \( r > r' \)

\[
G^R_m(r, r') = G_{jm}(r, r') J_{|m|}(kr') e^{im\theta_0} e^{-|m| r}
\]

which yields

\[
G_{jm}(r, r') = A(r') U[-v_m, |m| + 1, r^2/b^2] \left( \frac{r'}{b} \right)^{|m|} e^{-\frac{r'}{2b}}
\]

where we define \( v_m \) through \( E = \hbar a(2v_m + |m| + 1) \). Here, we have taken a small shortcut by introducing the Tricomi hypergeometric function \( U(a, b, z) \), which is the convergent solution for \( z \gg 1 \). Demanding that \( G^R_m(r, r') \) be regular at the origin yields the condition

\[
\lim_{r' \to 0} A(r') = \frac{2^{2|m|}\Gamma[-v_m]}{k^{|m|}}.
\]

Proceeding with general \( m \) is not attractive since the expressions for the lowest order terms are cumbersome. We therefore specialize to specific \( m \) values.

For \( m = 0 \), the spectrum should be universal according to the pseudopotential approach [3, 35]. The Green function approach has been discussed in a quasi-2D geometry with a tight transverse confinement [36]. First, consider the behavior of \( G_0(r, r') \) at the origin

\[
G_0(r, r') \to -i\pi + 2 \ln \left( \frac{kb}{2} \right) - \psi \left( \frac{1}{2} - \frac{k^2}{4} \right),
\]

for \( r, r' \to 0 \) \( (r > r') \), where \( \psi(x) \) is the digamma function. The scattering phase shift for \( m = 0 \) in 2D can be written [37]

\[
\cot \delta_0(k) = \frac{2}{\pi} \left( \psi + \ln \left[ \frac{ka_2^0}{2} \right] \right) + \frac{1}{2\pi} (r_e^2)^2 k^2,
\]

where \( a_2^0 \) is the 2D scattering length and \( r_e^2 \) is the effective range. \( \gamma \) is Euler’s constant. We have included the effective range term to discuss its effects below. Using equation (34), we arrive at the eigenvalue equation for the spectrum

\[
\gamma + \frac{1}{2} \psi (-v_0) + \frac{(r_e^2)^2}{b^2} \left( v_0 + \frac{1}{2} \right) = \ln \left[ \frac{b}{a_2^0} \right].
\]
In the case where \( r_s^2 = 0 \), this agrees with earlier works [3, 36, 35, 38, 39]. In the limit \( \frac{b}{a_{2D}} \to \infty \), the energy approaches the universal expression \( E = -\hbar^2 e^{-2\gamma}/2\mu[a_{2D}^2] \) (for \( r_s^2 = 0 \)) and represents the two-body bound state energy in the absence of the trap [40]. This is reasonable since the trap becomes irrelevant for large binding energy and small bound state size. The spectrum is shown in figure 4 for different values of \( r_s^2 \). We can see that effective range corrections will alter the energetics of the lowest state quite severely within this model. This is very similar to what is found for p-waves with range corrections in 3D [20].

The Green function method is particularly transparent when including higher order correction terms in comparison to the pseudopotential approach [3] or, equivalently, the Bethe–Peiels boundary condition [41, 38]. A mathematical formulation of pseudopotential approaches in any dimension and for any angular momentum was recently discussed by Stampfer and Wagner [42], which details the intricate problems of even dimensions in comparison to odd dimensions. The expression for the pseudopotential beyond lowest order is, however, involved. The Green function approach accomplishes these corrections in a simple manner.

Although the case of \( m = 0 \) was universal in the sense that the dependence on the details of the potential (through \( \tilde{\phi}(r) \) dropped out, there are a lot of indications that the case \( |m| > 0 \) is not so simple and will depend on short-distance physics. This has been pointed out by a number of authors and leads to the introduction of energy-dependent scattering lengths [43, 30, 20, 35] (see [44] for an alternative approach to pseudopotentials that can be applied in a well-defined manner in momentum space in both 2D and 3D). We now address this issue within the Green function approach for \( m = 1 \).

The expansion of \( G_1(r, r') \) is

\[
G_1(r, r') \to \frac{\pi kr}{2} \left[ -i + \frac{2}{\pi} \ln \left( \frac{kb}{2} \right) + \frac{2}{\pi (kb)^2} - \frac{1}{\pi} \psi (-\nu_1) \right].
\] (42)

Here, we have extracted a factor in front that agrees with \( J_1(kr) \) to lowest order in \( kr \). We find no other terms that depend explicitly on \( r \). In the \( m = 1 \) channel, it seems natural to define the
phase-shift relation that generalizes the $m = 0$ result as (see appendix B)
\[
\cot \delta_1(k) = \frac{2}{\pi} \left( \gamma + \ln \left( \frac{k a_{2D}^p}{2} \right) \right) + \frac{A}{(k a_{2D}^p)^2} + \frac{1}{2\pi} (r_e^p)^2 k^2
\] (43)

to order $k^2$ with $A$ being a dimensionless constant. The non-universal information about the two-body interaction potential is in fact carried by $A$ as pointed out in [45] and discussed further in appendix B. Let us consider the case when $A = 0$, which occurs if there is a bound state at zero energy in the $m = 1$ potential. In this case, we arrive at the very simple equation for the eigenspectrum
\[
\gamma + \frac{1}{2} \psi (-v_1) + \frac{r_e^2}{b^2} (v_1 + 1) + \frac{1}{4v_1 + 4} = \ln \left( \frac{b}{a_{2D}^p} \right).
\] (44)

The expression we obtain is very similar to the $m = 0$ case, except for the last term on the left-hand side that is the new piece. This extra term will vanish for large energies, but will be important around zero energy (where a bound state in free space resides). The spectrum is plotted in figure 5. We can see that the levels are pushed down compared to the $m = 0$ case, and a state reside at zero energy in the non-interacting $\frac{b}{a_{2D}^p} \to 0$ limit. A bound state appearing below the $m = 0$ ground state for $\frac{b}{a_{2D}^p} \to 0$ is not uncommon and also occurs for p-waves in 3D [20]. In the case of $A < 0$, there is a bound state with finite binding energy in the potential. However, we have checked that this only gives minor quantitative changes compared to the $A = 0$ in figure 5. Since $A = 0$ and $A < 0$ yield qualitatively the same spectra, we conclude that the extra term proportional to $k^{-2}$ makes little difference when the potential has a bound state (possibly at zero energy). Note that we are considering the zero-range limit for the potential, so there can be at most one bound state.

The $m = 1$ spectrum in a 2D trap was discussed in [35] and a spectrum can be found in figure 1 of [35]. We find good agreement with that result in the case when a bound state is present in the two-body potential, corresponding to $A < 0$ in equation (43). The level
rearrangement takes place at $a_{2D}^p \to 0$ as shown in figure 5 and there is a visible distortion of the manner in which this occurs similar to the examples in 3D of figures 1–3. These features can also be seen in [35]. When $A > 0$ in equation (43), we find that the lowest state shown in figure 5 does not diverge to minus infinite in binding energy for $a_{2D}^p \to 0$, but rather behaves similar to the higher lying states. This is consistent with the findings in [35], although we caution that the scattering area used to parameterize the strength in [35] can have both signs, while our $a_{2D}^p$ is defined to be positive.

To further explore the dependence of the $m = 1$ spectrum on the potential parameters, we show in figure 6 the results for a phase shift of the same form as the hard-sphere potential (appendix B) but with positive scattering length so that a bound state occurs. This is a somewhat unphysical potential but it helps illustrate the point that the spectrum is quite robust under changes in the value of $A$ (for $A \leq 0$) since figure 5 has $A = 0$, while figure 6 has $A = -4/\pi$ (see equation (B.7) ). Using a square well instead yields almost identical results and we have not plotted this case. In fact, the procedure of using a model potential to fix the phase shift used here is similar to the self-consistent energy-dependent pseudopotential methods employed for p-waves in 3D in [20]. This provides a significant improvement over the energy-independent pseudopotential in that case.

In the case of $|m| > 1$, we find that there are terms in $G_m(r, r')$ that do not vanish in the limit of $r, r' \to 0$ and that are not represented on the left-hand side of equation (34). We therefore conclude that the higher partial waves in 2D also yield non-universal spectra.

5. Conclusions and outlook

Using Green’s function techniques, we have derived the spectrum of two particles in an isotropic harmonic trap interacting through a potential that has a range that is much smaller
than the trap length scale in both three- and two-dimensional space. In the 3D case, the spectrum is universal, i.e. independent of the short-range details of the interaction, only for the s- and p-wave channels. For d-wave and beyond, there is a dependence on the short-distance physics. We derive a general criterion for when the universal expression is valid for higher angular momenta, which implies that one must be away from any resonances where the scattering length diverges. In the 2D case, only the s-wave spectrum is truly universal, but we demonstrated that the p-wave spectrum is not very sensitive to the exact details of the interaction as long as it can accommodate a two-body bound state.

The spectra in both 2D and 3D can be interpreted very nicely in terms of Zeldovich rearrangement, which occurs when adding a short-range (two-body interaction) to a long-range potential (trap) and tuning through a resonance of the short-range part. Including effective range corrections in the 3D s-wave channel shows that one can obtain a very rich set of rearrangement points depending on the background parameters of the resonance in the short-range interaction. In the realm of cold gases, this requires use of very narrow Feshbach resonances or very tight trapping conditions, both of which are currently beyond experimental capabilities but hopefully could be explored in future generation experiments.

It would be interesting to extend the current formalism to polar molecules for which external trapping potentials are of course also always present in experiments. A number of recent works [46] have explored the bound state structure of such systems but it not clear how much influence a harmonic trap or an optical lattice has on these few-body states.

Appendix A. Free Green’s functions

The free Green functions with the out-going wave boundary condition used in this paper are taken to satisfy the equation

\[
\left[ -\frac{\hbar^2 \nabla^2}{2 \mu} - E \right] G_0^E(r, r') = \frac{2\pi \hbar^2}{\mu} \delta(r - r'),
\]

where we define the corresponding momentum through \( E = \frac{\hbar^2 k^2}{2 \mu} \).

A.1. Three dimensions

The solution in 3D is

\[
G_0^E(r, r') = \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}.
\]

The partial wave expansion that we employ is written in terms of spherical Hankel functions of the first kind \( h_1^{(1)}(x) \) and spherical Bessel functions \( j_1(x) \). For \( r > r' \), we have

\[
G_0^E(r, r') = 4\pi i k \sum_{lm} j_l(kr') h_l^{(1)}(kr) Y_{lm}(\mathbf{r}) Y_{lm}^*(\mathbf{r'}),
\]

and for \( r < r' \), one interchanges the radial variables.

A.2. Two dimensions

The solution in 2D has been given by many authors, here we follow [34]. With the out-going wave boundary condition, the solution is

\[
G_0^E(r, r') = -\frac{i\mu}{2\hbar^2} H_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|),
\]

\[\]

14
where $H^{(1)}_m(x)$ is the first Hankel function of order $m$. The partial wave expansion of this Green function appears to be less accessible and we therefore write it explicitly here. Starting from the momentum space, we define $G^0_E = (E - H_0)^{-1}$. This implies that

$$
\langle r | G^E_0 | r' \rangle = \frac{1}{(2\pi)^2} \int d^2p \frac{e^{ip(r-r')}}{E - \frac{\hbar^2 p^2}{2\mu}}.
$$

(A.5)

where $p$ denotes the wave vector to be integrated over. Using the expansion

$$
e^{ikx \cos \phi} = \sum_{m=-\infty}^{\infty} i^{|m|} J^{|m|}(kx) e^{im\phi},
$$

(A.6)

where $J^m(x)$ is the Bessel function of order $m$, we can turn this into

$$
-\mu \pi \hbar^2 \sum_m \int_0^\infty dp \frac{J^{|m|}(pr) J^{|m|}(pr')} {p^2 - k^2}.
$$

(A.7)

This integral can be found in standard tables [47], and through analytical continuation, we obtain for $r > r' - i\mu^2 \hbar^2 \sum_m J^{|m|}(kr') H^{(1)}_m(kr)$.

(A.8)

With our normalization of Green’s function in equation (A.1), we finally end up with

$$
G^0_E(r, r') = i\pi \sum_m J^{|m|}(kr') H^{(1)}_m(kr).
$$

(A.9)

### Appendix B. 2D scattering

Scattering in 2D is complicated by the appearance of logarithmic terms in the typical wavefunction in the asymptotic region of large distance, which is a Neumann function $Y_m(x)$. Note that we are only interested in short-range potentials (vanishing for distances $r > r_0$) for which the asymptotic solution is the free one. We can therefore write the angular momentum $m$ scattering wavefunction $\Psi_m(r)$, for $r > r_0$ in the form

$$
\Psi_m(r) = A \left[ \cot \delta_m(k) J_m(kr) - Y_m(kr) \right],
$$

(B.1)

where $E = \hbar^2 k^2 / 2\mu$ and $N$ is a normalization constant. The phase shift $\delta_m(k)$ can be calculated from

$$
\cot \delta_m(k) = \frac{xY_m'(x) - y_m J_m(x)} {x J_m(x) - y_m Y_m(x)},
$$

(B.2)

where $x = kr_0$ and prime denotes derivative with respect to $x$. The logarithmic derivative is

$$
\gamma_m = \left. \frac{1} {\Psi_m(r)} \frac{d\Psi_m(r)} {dr} \right|_{r=r_0}.
$$

(B.3)

We discuss this in terms of an appropriately defined scattering length. Here, we follow the intuitively clear definition [48]

$$
\Psi_0(r) \rightarrow \ln \left[ \frac{r}{a_0} \right] \quad \text{and}
$$

$$
\Psi_m(r) \rightarrow r^m \left[ 1 - \left( \frac{a_m}{r} \right)^{2m} \right],
$$

(B.4)

for $m \geq 0$. 

15
The $m = 0$ case was studied by Verhaar et al \cite{37} who found the expression
\[
\cot \delta_0(k) = \frac{2}{\pi} \left( \gamma + \ln \left[ \frac{k a_0}{2} \right] \right) + \frac{1}{2\pi r^2} k^2 \tag{B.6}
\]
to second order in $k$. We expect a similar expression for the $m = 1$ phase shift, but very little can be found on this in the literature. To check this, we compute the exact expression for the hard-sphere potential and for the attractive square well potential. The hard sphere yields
\[
\cot \delta_1(k) = -\frac{4}{\pi (k r_0)^2} - \frac{3}{2\pi} + \frac{2}{\pi} \left( \gamma + \ln \left[ \frac{k r_0}{2} \right] \right), \tag{B.7}
\]
and the square well gives
\[
\cot \delta_1(k) = -\frac{12}{\pi (k r_0)^2} - \frac{11}{2\pi} + \frac{2}{\pi} \left( \gamma + \ln \left[ \frac{k r_0}{2} \right] \right), \tag{B.8}
\]
in the limit $2\mu r_0^2 V_0/\hbar^2 \to 0$, where the depth is $-V_0$. By using the definitions of the scattering length $a_m$ above, we find $a_1^s = r_0^s$ for the hard sphere and $a_1^s = \frac{r_0^s}{2}$ for the square well. The choice of sign for $a_1$ is not given directly by these relations. In the regime where there is a bound states in the potential, the definition above implies $a_m > 0$. Since we know that the hard-sphere potential should not hold a bound state, a suitable choice is $a_1 = -r_0$, and similarly, for the square-well potential in the limit $2\mu r_0^2 V_0/\hbar^2 \to 0$, where the centrifugal barrier hinders the formation of a bound state \cite{49}. We will be interested in the regime $a_1 > 0$ only, as it is nicely comparable to the $m = 0$ case. To approach the zero-range limit with a bound state always present for the square well, one needs to take the limit of $r_0 \to 0$ and $-V_0 \to \infty$ in a manner that keeps $2\mu r_0^2 V_0/\hbar^2$ at or above the critical limit for the appearance of a bound state.

From the discussion above, we obtain the suggestive expression for the phase shift:
\[
\cot \delta_1(k) = \frac{A}{(k a_1)^2} + B + \frac{2}{\pi} \left( \gamma + \ln \left[ \frac{k a_1}{2} \right] \right), \tag{B.9}
\]
where $A$ and $B$ are the potential-dependent low-energy constants. We find that the structure of $\cot \delta_1(k)$ is very similar to the $m = 0$ case, except that there is an added $k^{-2} \propto E^{-1}$ term. The leading divergence in the corresponding scattering amplitude is therefore a pole rather than the logarithm as for $m = 0$. This was pointed out in \cite{45}. In the main text, we have shown that in the presence of a harmonic trap, it does not make much difference whether the leading $E^{-1}$ term is included or not when calculating the two-body spectrum in the presence of a bound state. This can be seen from comparison of figure 5 (with $A = 0$) and figure 6 (with $A < 0$). However, in the case with $A > 0$, there is no bound state as discussed in the main text.

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