Energetics of three particles near a three-body resonance

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• One particle in 6 dimensions
• Three particles in the 3 dimensional box
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Introduction

• Ultracold atoms: small collision energies (compared to the Van der Waals energy); large de Broglie wave lengths (compared to the Van der Waals range).

• Low-energy nucleons/nuclei are similar
Introduction

• Ultracold atoms: small collision energies (compared to the Van der Waals energy); large de Broglie wave lengths (compared to the Van der Waals range).

• Low-energy nucleons/nuclei are similar

Develop a general approach for a few particles, treating $E$ and $1/l$ as small parameters

$E$: energy $l$: size of system
A general framework for few-body physics in the ultracold regime

Consider any number of objects, in any dimension, with generic interactions, colliding at a small energy:

\[ H \psi = E \psi \]

In a region of configuration space small compared to the de Broglie wave length associated with \( E \):

\[
\psi = \sum_{\mu} c_{\mu} (\phi^{(\mu)} + Ef^{(\mu)} + E^2 g^{(\mu)} + \cdots )
\]

where

\[ H \phi^{(\mu)} = 0 \quad H f^{(\mu)} = \phi^{(\mu)} \quad H g^{(\mu)} = f^{(\mu)} \quad \cdots \]

\( \phi^{(\mu)}, f^{(\mu)}, g^{(\mu)}, \cdots \): special wave functions

see, eg, Tan, PRA 2008
Why study resonances

• Ultracold atoms are usually weakly interacting

• A lot are known:
  use two-body scattering length, two-body effective range, three-body scattering hypervolume, etc as effective interaction parameters

• Turn to resonances: system strongly interacting, and much more interesting

• But a lot are known about TWO-body resonances

• So let’s turn to THREE-BODY RESONANCES
Why study three-body resonances?

- [Definition]
  If three particles have a bound state near zero energy, we say they are near a three-body resonance

- Strongly interacting and interesting

- Applications in ultracold atoms near three-body resonances, and three-body nuclear halo states

- Applications in other systems (e.g., excitons, other particles)
Textbook wisdom

Three-body problem often cannot be solved analytically (famous example: the motion of 3 gravitating celestial bodies may display chaos)

But, let us study 3-body problem analytically

Our trick: study the wave functions at small collision energies & large inter-particle distances
Three-body Schrödinger equation

Consider 3 bosons with interactions that are translationally, rotationally, and Galilean invariant, and short-ranged, fine-tuned such that there is a bound state with zero energy and zero orbital angular momentum.

\[ H_3 \psi = E \psi \]

\[ (H_3 \psi)_{k_1 k_2 k_3} = \frac{k_1^2 + k_2^2 + k_3^2}{2} \psi_{k_1 k_2 k_3} + \frac{1}{2} \int_{k'} U_{k_1 k_2 k' k'' k_3} \psi_{k' k'' k_3} + \frac{1}{2} \int_{k'} U_{k_2 k_3 k' k'' k_3} \psi_{k_1 k' k'' k_3} \]

\[ + \frac{1}{2} \int_{k'} U_{k_3 k_1 k' k'' k_2} \psi_{k' k'' k_2} + \frac{1}{6} \int_{k_1' k_2'} U_{k_1 k_2 k_3 k_1' k_2' k_3' \psi_{k_1' k_2' k_3'}} \]

where \( \int_{k'} = \int \frac{d^3 k'}{(2\pi)^3}, \quad \int_{k_1' k_2'} = \int \frac{d^3 k_1'}{(2\pi)^3} \frac{d^3 k_2'}{(2\pi)^3} \)

\( (m = \hbar = 1) \)
Two-body special wave functions

\[ H_2\psi = E\psi \]

\[ (H_2\psi)_k = k^2\psi_k + \frac{1}{2} \int \frac{d^3k'}{(2\pi)^3} U_{k,-k,k',-k'}\psi_{k'} \]

In the ultracold regime, \( E \) is small. May expand the wave function as

\[ \psi_k = \phi_k + Ef_k + E^2g_k + \cdots \]

\[ H\phi_k = 0 \quad Hf_k = \phi_k \quad Hg_k = f_k \]

Outside the range of interaction, we have

\[ \phi(r) = 1 - a/r \quad f(r) = -r^2/6 + ar/2 - ar_s/2 \]

\[ \phi_{\hat{n}}^{(d)}(r) = (r^2/15 - 3a_d/r^3)P_2(\hat{n} \cdot \hat{r}) \]
Three-body special wave functions

\[ H_3 \psi = E \psi \]

In the ultracold regime, \( E \) is small. May expand the wave function as

\[ \psi = \phi^{(3)} + Ef^{(3)} + E^2g^{(3)} + \cdots \]

where \( \phi_{k_1 k_2 k_3}^{(3)} \), \( f_{k_1 k_2 k_3}^{(3)} \), \( g_{k_1 k_2 k_3}^{(3)} \), etc, are special wave functions, and serve as building blocks of the wave functions at arbitrary energies.

\[ H_3 \phi^{(3)} = 0 \]
\[ H_3 f^{(3)} = \phi^{(3)} \]
\[ H_3 g^{(3)} = f^{(3)} \]
\[ \cdots \]
Once we know the special wave functions, $\phi_{k_1k_2k_3}^{(3)}$, $f_{k_1k_2k_3}^{(3)}$, $g_{k_1k_2k_3}^{(3)}$, etc, we know ALL the details of three-body effective interactions at low energy.

The effective parameters such as the three-body scattering hypervolume appear in the large-distance or low-momentum expansions of these functions.
The special wave function $\phi^{(3)}$

When $s_1$, $s_2$, $s_3$ are all large,

$$\phi^{(3)}(r_1 r_2 r_3) \propto 1 + \left[ \sum_{i=1}^{3} -\frac{a}{s_i} + \frac{4a^2\theta_i}{\pi R_i s_i} - \frac{2w a^3}{\pi \rho^2 s_i} + \frac{8\sqrt{3} w a^4 (\ln \frac{\rho}{|a|} + \gamma - 1 - \theta_i \cot 2\theta_i)}{\pi^2 \rho^4} \right] - \frac{\sqrt{3} D}{8\pi^3 \rho^4} + O(\rho^{-5})$$

Tan, PRA 2008

At a three-body resonance, $D \rightarrow \pm \infty$, and

$$\phi^{(3)}(r_1 r_2 r_3) \propto \frac{1}{\rho^4} + O(\rho^{-5})$$

which is also the wave function of the shallow three-body bound state
The special wave function $\phi^{(3)}$

The formula $\phi^{(3)}(r_1 r_2 r_3) \propto \frac{1}{\rho^4} + O(\rho^{-5})$ at large distances

corresponds to $\phi^{(3)}_{q_1 q_2 q_3} \propto \frac{2}{q_1^2 + q_2^2 + q_3^2} + O(q^{-1})$
at small momenta
The special wave function $\phi^{(3)}$

There are small-momentum asymptotic expansions for

$$\phi^{(3)}_{q_1 q_2 q_3} \text{ and } \phi^{(3)}_{q, -q/2 + k, -q/2 - k}$$

where q’s are small but k is not.

Solving the exact Schrödinger equation, we can refine the two asymptotic expansions back and forth, in a zig-zag manner.
The special wave function $\phi^{(3)}$

Asymptotic expansions at small $q$’s:

$$\phi^{(3)}_{q,-q/2+k,-q/2-k} = \left[ -\frac{\sqrt{3}}{8\pi} q + \frac{a}{\sqrt{3} \pi^2} q^2 \ln(q|a|) + \left( \frac{9 + 2\sqrt{3} \pi}{72\pi^2} a^2 + \frac{3\sqrt{3}}{64\pi} ar_s \right) q^3 \right] \phi_k$$

$$+ \frac{3\sqrt{3}}{32\pi} q^3 f_k + d_k + q^2 d^{(2)}_{qk} + O(q^4)$$

$$\phi^{(3)}_{q_1 q_2 q_3} = \frac{2}{q_1^2 + q_2^2 + q_3^2} \left\{ 1 + \sum_{i=1}^{3} \left[ \frac{\sqrt{3}}{2} a q_i - \frac{4}{\sqrt{3} \pi} a^2 q_i^2 \ln(q_i|a|) \right] \right\} + \chi_0 + O(q)$$

$a$: two-body scattering length

$r_s$: two-body effective range

These expansions will be essential in the ultracold physics of three or more such particles
The special wave function $f^{(3)}$

$$H_3 f^{(3)} = \phi^{(3)}$$

At small q’s, we get

$$f^{(3)}_{q_1q_2q_3} = r_3 (2\pi)^6 \delta(q_1)\delta(q_2) + O(q^{-5}),$$

where $r_3$ is the three-body effective range. It’s the MOST IMPORTANT three-body parameter at a resonance (its dimension: 1/length^2).

Using the Schrödinger equation, we get

$$\int_{k_1k_2} |\phi^{(3)}_{k_1k_2k_3}|^2 = -r_3$$
$r_3$ as a probability constant

From the formula

$$\int_{k_1 k_2} \left| \phi^{(3)}_{k_1 k_2 k_3} \right|^2 = -r_3,$$

we find

$$\int_{\rho<\eta} d^3 r d^3 R \left| \phi^{(3)} (r/2, -r/2, R) \right|^2 \propto 16\sqrt{3} \pi^3 |r_3| - \frac{1}{\eta^2} + O(\eta^{-3})$$

at a large cutoff hyperradius $\eta$
The special wave function $f^{(3)}$

$$f^{(3)}_{q,-q/2+k,-q/2-k} = \left[ r_3(2\pi)^3 \delta(q) - \frac{8\pi a r_3}{q^2} + \left(4\pi wa^2 r_3 + \frac{\sqrt{3}}{12\pi}\right) \frac{1}{q} + \left(16wa^3 r_3 - \frac{a}{2\sqrt{3} \pi^2}\right) \ln(|q|a) \right]$$

$$+ \left[24\sqrt{3} wa^4 r_3 + \frac{a^2}{4\pi^2}\right] q \ln(|q|a) + c_1 q \right] \hat{\phi}_k - \left(3\pi wa^2 r_3 + \frac{3\sqrt{3}}{16\pi}\right) q f_k$$

$$+ \left[10\pi a r_3 - 10\pi(2\pi - 3\sqrt{3}) a^2 r_3 q\right] \phi^{(d)}_{qk} + \hat{d}_k + O(q^2)$$

$$f^{(3)}_{q_1 q_2 q_3} = r_3(2\pi)^6 \delta(q_1) \delta(q_2) + \left(\frac{2}{q_1^2 + q_2^2 + q_3^2}\right)^2 \left\{ 1 + \sum_{i=1}^3 \left[ \frac{\sqrt{3}}{2} a q_i - \frac{4}{\sqrt{3} \pi} a^2 q_i^2 \ln(|q_i|a) \right] \right\}$$

$$+ \frac{2}{q_1^2 + q_2^2 + q_3^2} \sum_{i=1}^3 \left[ -4\pi a r_3(2\pi)^3 \delta(q_i) + \frac{32\pi^2 a^2 r_3}{q_i^2} - \left(16\pi^2 wa^3 r_3 + \frac{a}{\sqrt{3}}\right) \frac{1}{q_i} \right.$$

$$\left. + \left(-64\pi wa^4 r_3 + \frac{2}{\sqrt{3} \pi} a^2\right) \ln(|q_i|a) \right]$$

$$+ u_0 r_3 \sum_{i=1}^3 \left[ (2\pi)^3 \delta(q_i) - \frac{8\pi a}{q_i^2}\right] + O(q^{-1}),$$

$$c_1 \equiv \left[ -8\left(\sqrt{3} - \frac{\pi}{3}\right) wa^4 - \frac{3}{2} \pi wa^3 r_s\right] r_3 + \left(\frac{1}{4\pi^2} - \frac{1}{12\sqrt{3} \pi}\right) a^2 - \frac{3\sqrt{3}}{32\pi} ar_s$$
Now place the 3 particles in a large cubic box, and impose the periodic boundary condition

![Diagram of a large cubic box with three particles](image)

Question: how does the energy scale with $L$?

My previous conjecture: 

$$E = -\frac{\#}{|r_3|L^4} + O(L^{-5})$$

But this turns out to be incorrect :( 

And even the question itself is slightly incorrect!
Before solving the above problem, consider an analogous, but easier problem:

**ONE body in 6 dimensions, at a resonance**

\[-\nabla^2 \psi(r) + \int d^6r' V(r, r') \psi(r') = E \psi(r)\]

(V: rotationally invariant, and short-ranged (vanishes outside a finite 6d sphere around the origin)

Effective-range expansion for the \(s\)-wave phase shift \(\delta\):

\[k^4 \cot \delta = -\frac{1}{a} + \frac{1}{2} r_s k^2 + \frac{2}{\pi} k^4 \ln(kr_s') + O(k^6)\]

\(r_s\): effective range (dimension: 1/length^2)

\(a = \pm \infty\) at resonance
ONE body in 6 dimensions at a resonance

\[-\nabla^2 \psi(r) + \int d^6 r' V(r, r') \psi(r') = E \psi(r)\]

s-wave special wave functions

In real space (outside the range of potential):

\[
\phi(r) = \frac{1}{4\pi^3 r^4}
\]

\[
f(r) = \frac{r_s}{256\pi^2} + \frac{1}{16\pi^3 r^2}
\]

In momentum space:

\[
\phi_k = \frac{1}{k^2} + \text{(smooth function of } k\text{)}
\]

\[
f_k = \frac{r_s}{256\pi^2} (2\pi)^6 \delta(k) + \frac{1}{k^4} + \text{(smooth function of } k\text{)}
\]
ONE body in 6 dimensions at a resonance

Now impose the periodic boundary condition:

\[ \psi(x_1 + L, x_2, x_3, x_4, x_5, x_6) = \cdots = \psi(x_1, x_2, x_3, x_4, x_5, x_6) \]

Result:

\[
E = \pm \frac{16\pi}{\sqrt{|r_s|}} L^{-3} + \frac{32\alpha_1}{r_s} L^{-4} \pm \frac{32(\alpha_1^2 - 4\alpha_2)}{\pi |r_s|^{3/2}} L^{-5} + O(L^{-6})
\]

There are TWO states with energies close to zero!

The energy of each state scales like \(1/L^3\) at large \(L\), rather than \(1/L^4\) as I previously conjectured.

\[
\alpha_1 \equiv \sum_{n \neq 0} \frac{1}{n^2} = -3.37968478344314798726129011
\]

\[
\alpha_2 \equiv \sum_{n \neq 0} \frac{1}{n^4} = \pi \alpha_1
\]
ONE body in 6 dimensional box

When $V=0$, we know the energy-momentum eigenstates:

$$E = \frac{(2\pi|n|)^2}{L^2} \quad p = \frac{2\pi n}{L}$$

Ground state: nondegenerate
First excited state: 12-fold degenerate

But at resonance, there are TWO low energy states, with energies

$$E_- \approx -\frac{16\pi}{\sqrt{|r_s|}} L^{-3} \quad E_+ \approx +\frac{16\pi}{\sqrt{|r_s|}} L^{-3}$$

So where does the positive energy state, $E_+$, come from?

Answer: it has evolved from the equal superposition of the 12 first excited states.

confirmed using a separable potential $V_{kk'} = -\eta e^{-\frac{k^2}{2}} e^{-\frac{k'^2}{2}}$
Now return to the 3 particles in the 3-dimensional box

Strategy: in the momentum space, expand the wave function and energy in powers of $\varepsilon \equiv 1/L$:

$$
\psi_{k_1 k_2 k_3} = R^{(0)}_{k_1 k_2 k_3} + R^{(1)}_{k_1 k_2 k_3} + R^{(2)}_{k_1 k_2 k_3} + \cdots
$$

$$
\psi_{q, -q/2+k, -q/2-k} = S^{(0)}_k q + S^{(1)}_k q + S^{(2)}_k q + \cdots
$$

$$
\psi_{q_1 q_2 q_3} = T^{(-3)}_{q_1 q_2 q_3} + T^{(-2)}_{q_1 q_2 q_3} + T^{(-1)}_{q_1 q_2 q_3} + \cdots
$$

$$
E = E^{(3)} + E^{(4)} + E^{(5)} \cdots
$$

where q’s are of order $\varepsilon$, and k’s are independent of $\varepsilon$, and

$$X^{(s)} \sim \varepsilon^s$$
3 particles at a resonance in the 3-dimensional box

Solving the Schrödinger equation perturbatively in powers of $\varepsilon$, I find, eg,

\[
R_{k_1k_2k_3}^{(0)} = \phi_{k_1k_2k_3}^{(3)}
\]

\[
R_{k_1k_2k_3}^{(3)} = E^{(3)} f_{k_1k_2k_3}^{(3)} + \text{(terms that are less singular at or}
\]

\[
T_{q_1q_2q_3}^{(-3)} = j \varepsilon^3 (2\pi)^6 \delta(q_1) \delta(q_2)
\]

\[
S_k^{(0)q} = (2\pi\varepsilon)^3 j \delta(q) \phi_k + d_k \sum_n (2\pi\varepsilon)^3 \delta(q - 2\pi\varepsilon n)
\]

\[
(12\pi a - E^{(3)} \varepsilon^{-3}) j = 1
\]

\[
j = E^{(3)} \varepsilon^{-3} r_3
\]
3 particles at a resonance in the 3-dimensional box

Solving the equations

$$(12\pi a - E^{(3)} \epsilon^{-3}) j = 1$$

$$j = E^{(3)} \epsilon^{-3} r_3$$

we get TWO low energy states, with energies

$$E = \frac{6\pi a \pm \sqrt{(6\pi a)^2 + \frac{1}{|r_3|}}}{L^3} + O(L^{-4})$$
3 particles at a resonance in the 3-dimensional box

\[ E = \frac{6\pi a \pm \sqrt{(6\pi a)^2 + \frac{1}{|r_3|}}}{L^3} + O(L^{-4}) \]

If the two scattering length \( a = 0 \),

\[ E \approx \pm \frac{1}{\sqrt{|r_3|} L^3} \]

analogous to the one body at a resonance in 6-dimensional box
3 particles at a resonance in the 3-dimensional box

\[ E = \frac{6\pi a \pm \sqrt{(6\pi a)^2 + \frac{1}{|r_3|}}}{L^3} + O(L^{-4}) \]

If the resonance is very narrow \((r_3 \to -\infty)\),

\[ E_1 \approx \frac{12\pi a}{L^3} \quad (3\text{-body state with an energy mainly due to two-body interactions}) \]

\[ E_2 \approx -\frac{1}{12\pi a|r_3|L^3} \quad (another \ 3\text{-body state}) \]
Other results

If the interaction is slightly more attractive than the critical interaction, so that $D$ is large and positive, there is a shallow three-body bound state with energy

$$E \approx -\frac{1}{|r_3|D}$$

But if the interaction is slightly less attractive than the critical interaction, so that $D$ is large and negative, there is a metastable three-body state with energy

$$E \approx +\frac{1}{|r_3D|} - i(\text{small imaginary part})$$
Summary

• Determined the special three-body wave functions at a three-body resonance in powers of $1/\{\text{size of the system}\}$.

• Defined the three-body effective range in terms of the special wave functions.

• Determined the low lying energy eigenstates in a large periodic volume. Found TWO such states.
Future directions on this subject

• Three particles at a three-body resonance in a harmonic trap

• Definition of three-body effective range away from resonance

• More precise formula for the three-body bound state (or metastable state) energy slightly off resonance

• Three-body resonances in the presence of long-range Van der Waals potential

• Three-body resonances for identical fermions

• ...