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Energetics of three particles near a three-body resonance

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Outline

- Introduction
- Special wave functions for three particles at a resonance
- One particle in 6 dimensions
- Three particles in the 3 dimensional box
- Other results
- Summary

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

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  are similar

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

E: energy l: size of system

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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:

$$\psi = \sum_{\mu} c_{\mu}(\phi^{(\mu)} + E f^{(\mu)} + E^2 g^{(\mu)} + \cdots)$$

where

$$H\phi^{(\mu)} = 0 \qquad H f^{(\mu)} = \phi^{(\mu)} \qquad H g^{(\mu)} = f^{(\mu)} \qquad \ldots$$

$\phi^{(\mu)}, f^{(\mu)}, g^{(\mu)}, \cdots$: 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 (eg, 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.

$$H_3\psi = E\psi$$

$$(H_3\psi)_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \frac{k_1^2+k_2^2+k_3^2}{2}\psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \frac{1}{2}\int_{\mathbf{k}'} U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}'\mathbf{k}''}\psi_{\mathbf{k}'\mathbf{k}''\mathbf{k}_3} + \frac{1}{2}\int_{\mathbf{k}'} U_{\mathbf{k}_2\mathbf{k}_3\mathbf{k}'\mathbf{k}''}\psi_{\mathbf{k}_1\mathbf{k}'\mathbf{k}''}$$

$$+\frac{1}{2}\int_{\mathbf{k}'} U_{\mathbf{k}_3\mathbf{k}_1\mathbf{k}'\mathbf{k}''}\psi_{\mathbf{k}'\mathbf{k}_2\mathbf{k}''} + \frac{1}{6}\int_{\mathbf{k}_1'\mathbf{k}_2'} U_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}\psi_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3'}$$

where $\int_{\mathbf{k}'} \equiv \int \frac{d^3k'}{(2\pi)^3}, \quad \int_{\mathbf{k}_1'\mathbf{k}_2'} \equiv \int \frac{d^3k_1'}{(2\pi)^3}\frac{d^3k_2'}{(2\pi)^3}$ $(m = \hbar = 1)$

Two-body special wave functions

$$H_2\psi = E\psi$$

$$(H_2\psi)_{\mathbf{k}} = k^2\psi_{\mathbf{k}} + \frac{1}{2}\int \frac{d^3k'}{(2\pi)^3} U_{\mathbf{k},-\mathbf{k},\mathbf{k}',-\mathbf{k}'}\psi_{\mathbf{k}'}$$

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

$$\psi_{\mathbf{k}} = \phi_{\mathbf{k}} + E f_{\mathbf{k}} + E^2 g_{\mathbf{k}} + \cdots$$

$$H\phi_{\mathbf{k}} = 0 \qquad H f_{\mathbf{k}} = \phi_{\mathbf{k}} \qquad H g_{\mathbf{k}} = f_{\mathbf{k}} \qquad \ldots\ldots$$

Outside the range of interaction, we have

$$\phi(\mathbf{r}) = 1 - a/r \qquad f(\mathbf{r}) = -r^2/6 + ar/2 - ar_s/2$$

$$\phi^{(d)}_{\hat{\mathbf{n}}}(\mathbf{r}) = (r^2/15 - 3a_d/r^3)P_2(\hat{\mathbf{n}}\cdot\hat{\mathbf{r}})$$

Three-body special wave functions

$$H_3\psi = E\psi$$

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

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

where $\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, $f^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, $g^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, etc, are special wave functions, and serve as *building blocks* of the wave functions at arbitrary energies.

$$H_3\phi^{(3)} = 0$$

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

$$H_3 g^{(3)} = f^{(3)}$$

...

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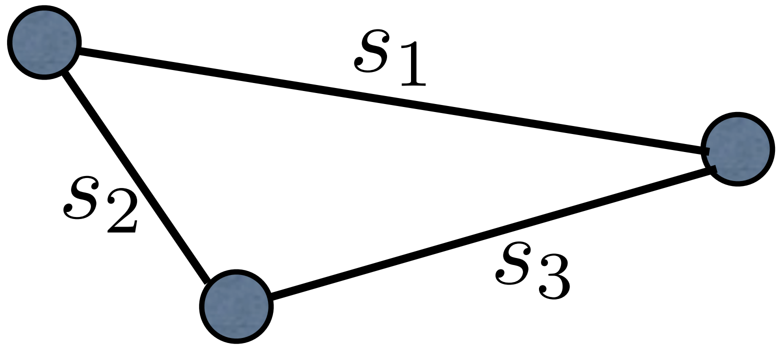
Three-body special wave functions

Once we know the special wave functions,
$\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, $f^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, $g^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$, 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 $\phi^{(3)}$



$$w = \frac{4\pi}{3} - \sqrt{3}$$

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

$$\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) \propto 1 + \Big[\sum_{i=1}^{3} -\frac{a}{s_i} + \frac{4a^2\theta_i}{\pi R_i s_i} - \frac{2wa^3}{\pi\rho^2 s_i} + \frac{8\sqrt{3}\,wa^4(\ln\frac{\rho}{|a|} + \gamma - 1 - \theta_i\cot 2\theta_i)}{\pi^2\rho^4}\Big] - \frac{\sqrt{3}\,D}{8\pi^3\rho^4} + O(\rho^{-5})$$

Tan, PRA 2008

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

$$\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) \propto \frac{1}{\rho^4} + O(\rho^{-5})$$

which is also the wave function of the shallow three-body bound state

The special wave function $\phi^{(3)}$

The formula $\phi^{(3)}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) \propto \dfrac{1}{\rho^4} + O(\rho^{-5})$ at large distances

corresponds to $\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} \propto \dfrac{2}{q_1^2 + q_2^2 + q_3^2} + O(q^{-1})$
at small momenta

The special wave function $\phi^{(3)}$

There are small-momentum asymptotic expansions for

$$\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} \text{ and } \phi^{(3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}}$$

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:

$$\phi^{(3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}} = \Big[-\frac{\sqrt{3}}{8\pi}q + \frac{a}{\sqrt{3}\,\pi^2}q^2\ln(q|a|) + \Big(\frac{9+2\sqrt{3}\,\pi}{72\pi^2}a^2 + \frac{3\sqrt{3}}{64\pi}ar_s\Big)q^3\Big]\phi_{\mathbf{k}}$$
$$+\frac{3\sqrt{3}}{32\pi}q^3 f_{\mathbf{k}} + d_{\mathbf{k}} + q^2 d^{(2)}_{\hat{\mathbf{q}}\mathbf{k}} + O(q^4)$$

$$\phi^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \frac{2}{q_1^2+q_2^2+q_3^2}\Big\{1+\sum_{i=1}^{3}\Big[\frac{\sqrt{3}}{2}aq_i - \frac{4}{\sqrt{3}\,\pi}a^2q_i^2\ln(q_i|a|)\Big]\Big\} + \chi_0 + O(q)$$

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

$$f^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = r_3 (2\pi)^6 \delta(\mathbf{q}_1)\delta(\mathbf{q}_2) + O(q^{-5}),$$

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

$$\int_{\mathbf{k}_1\mathbf{k}_2} \left|\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}\right|^2 = -r_3$$

r_3 as a probability constant

From the formula

$$\int_{\mathbf{k}_1\mathbf{k}_2} \left|\phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}\right|^2 = -r_3,$$

we find

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

at a large cutoff hyperradius η

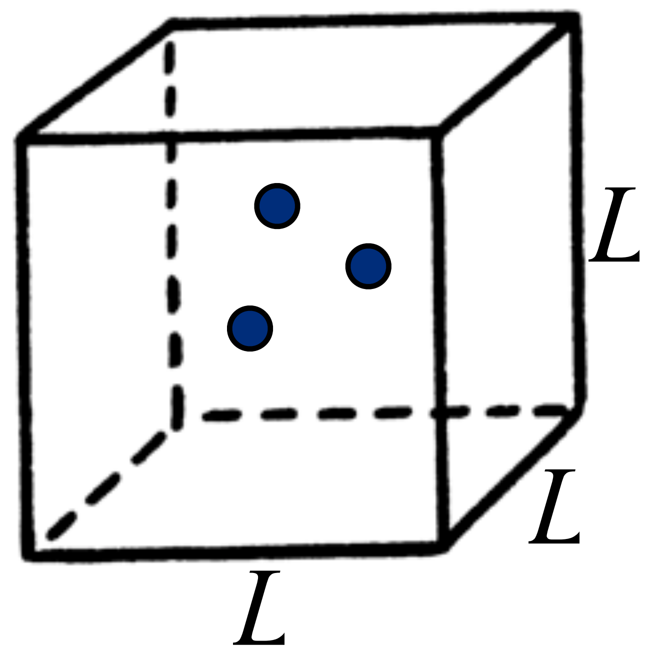
The special wave function $f^{(3)}$

$$f^{(3)}_{\mathbf{q},-\mathbf{q}/2+\mathbf{k},-\mathbf{q}/2-\mathbf{k}} = \Big[r_3(2\pi)^3\delta(\mathbf{q}) - \frac{8\pi a r_3}{q^2} + \Big(4\pi w a^2 r_3 + \frac{\sqrt{3}}{12\pi}\Big)\frac{1}{q} + \Big(16 w a^3 r_3 - \frac{a}{2\sqrt{3}\,\pi^2}\Big)\ln(q|a|)$$
$$+\Big(24\sqrt{3}\,w a^4 r_3 + \frac{a^2}{4\pi^2}\Big)q\ln(q|a|) + c_1 q\Big]\phi_{\mathbf{k}} - \Big(3\pi w a^2 r_3 + \frac{3\sqrt{3}}{16\pi}\Big)q f_{\mathbf{k}}$$
$$+\Big[10\pi a r_3 - 10\pi(2\pi - 3\sqrt{3}\,)a^2 r_3 q\Big]\phi^{(d)}_{\hat{\mathbf{q}}\mathbf{k}} + \hat{d}_{\mathbf{k}} + O(q^2)$$

$$f^{(3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = r_3(2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2) + \Big(\frac{2}{q_1^2+q_2^2+q_3^2}\Big)^2\Big\{1 + \sum_{i=1}^{3}\Big[\frac{\sqrt{3}}{2}a q_i - \frac{4}{\sqrt{3}\,\pi}a^2 q_i^2\ln(q_i|a|)\Big]\Big\}$$
$$+\frac{2}{q_1^2+q_2^2+q_3^2}\sum_{i=1}^{3}\Big[-4\pi a r_3(2\pi)^3\delta(\mathbf{q}_i) + \frac{32\pi^2 a^2 r_3}{q_i^2} - \Big(16\pi^2 w a^3 r_3 + \frac{a}{\sqrt{3}}\Big)\frac{1}{q_i}$$
$$+\Big(-64\pi w a^4 r_3 + \frac{2}{\sqrt{3}\,\pi}a^2\Big)\ln(q_i|a|)\Big]$$
$$+u_0 r_3\sum_{i=1}^{3}\Big[(2\pi)^3\delta(\mathbf{q}_i) - \frac{8\pi a}{q_i^2}\Big] + O(q^{-1}),$$

$$c_1 \equiv \Big[-8\Big(\sqrt{3} - \frac{\pi}{3}\Big)w a^4 - \frac{3}{2}\pi w a^3 r_s\Big]r_3 + \Big(\frac{1}{4\pi^2} - \frac{1}{12\sqrt{3}\,\pi}\Big)a^2 - \frac{3\sqrt{3}}{32\pi}a r_s$$

Now place the 3 particles in a large cubic box, and impose the periodic boundary condition



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

$$-\nabla^2\psi(\mathbf{r}) + \int d^6r' V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}') = E\psi(\mathbf{r})$$

$(2m = \hbar = 1)$

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

Effective-range expansion for the s-wave phase shift δ:

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

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

$a = \pm\infty$ at resonance

ONE body in 6 dimensions at a resonance

$$-\nabla^2\psi(\mathbf{r}) + \int d^6r' V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}') = E\psi(\mathbf{r})$$

s-wave special wave functions

In real space (outside the range of potential):

$$\phi(\mathbf{r}) = \frac{1}{4\pi^3 r^4}$$

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

In momentum space:

$$\phi_{\mathbf{k}} = \frac{1}{k^2} + (\text{smooth function of } \mathbf{k})$$

$$f_{\mathbf{k}} = \frac{r_s}{256\pi^2}(2\pi)^6\delta(\mathbf{k}) + \frac{1}{k^4} + (\text{smooth function of } \mathbf{k})$$

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.

$$\alpha_1 \equiv \sum_{\mathbf{n}\neq 0}' \frac{1}{n^2} = -3.37968478344314798726129011$$

$$\alpha_2 \equiv \sum_{\mathbf{n}\neq 0}' \frac{1}{n^4} = \pi\alpha_1$$

ONE body in 6 dimensional box

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

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

Ground state: nondegenerate → energy gap $\sim 1/L^2$

First excited state: 12-fold degenerate →

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

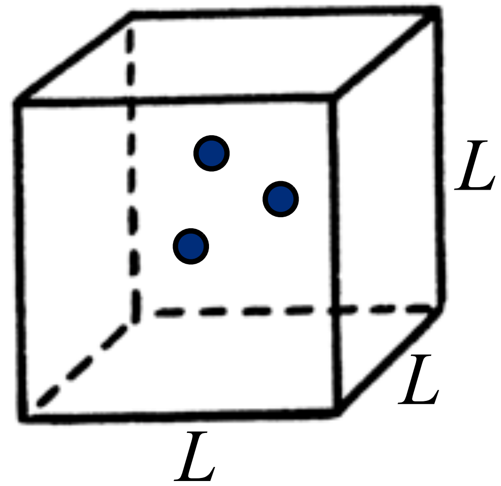
$$E_- \approx -\frac{16\pi}{\sqrt{|r_s|}} L^{-3} \qquad E_+ \approx +\frac{16\pi}{\sqrt{|r_s|}} L^{-3}$$

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 $V_{\mathbf{k}\mathbf{k}'} = -\eta e^{-\frac{k^2}{2}} e^{-\frac{k'^2}{2}}$

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 ε ≡ 1/L:

$$\psi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \mathcal{R}^{(0)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \mathcal{R}^{(1)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \mathcal{R}^{(2)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + \cdots$$

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

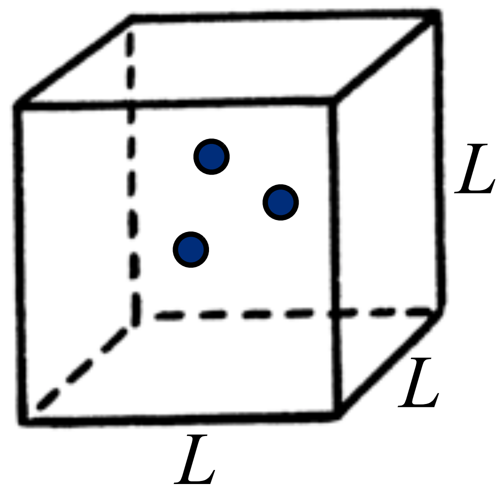
$$\psi_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = \mathcal{T}^{(-3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} + \mathcal{T}^{(-2)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} + \mathcal{T}^{(-1)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} + \cdots$$

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

where q's are of order ε, and k's are independent of ε, and

$$X^{(s)} \sim \varepsilon^s$$

3 particles at a resonance in the 3-dimensional box



Solving the Schrödinger equation perturbatively in powers of ε, I find, eg,

$$\mathcal{R}^{(0)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = \phi^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}$$

$$\mathcal{R}^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} = E^{(3)} f^{(3)}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} + (\text{terms that are less singular at or}$$

$$\mathcal{T}^{(-3)}_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3} = j\epsilon^3(2\pi)^6\delta(\mathbf{q}_1)\delta(\mathbf{q}_2)$$

$$\mathcal{S}^{(0)\mathbf{q}}_{\mathbf{k}} = (2\pi\epsilon)^3 j\delta(\mathbf{q})\phi_{\mathbf{k}} + d_{\mathbf{k}}\sum_{\mathbf{n}}(2\pi\epsilon)^3\delta(\mathbf{q} - 2\pi\epsilon\mathbf{n})$$

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

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

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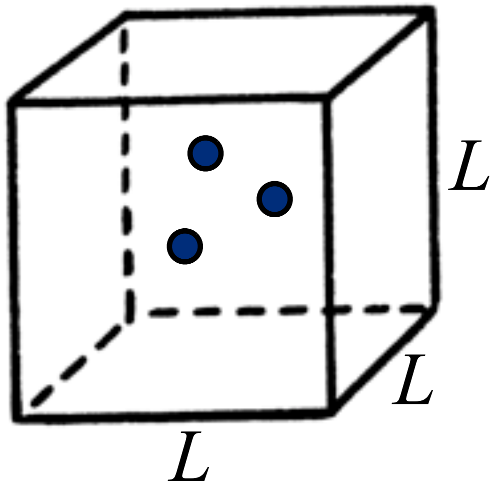
3 particles at a resonance in the 3-dimensional box



Solving the equations

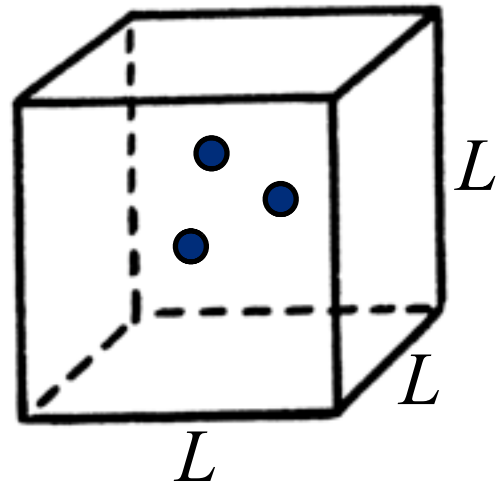
$$(12\pi a - E^{(3)}\epsilon^{-3})j = 1$$

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

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



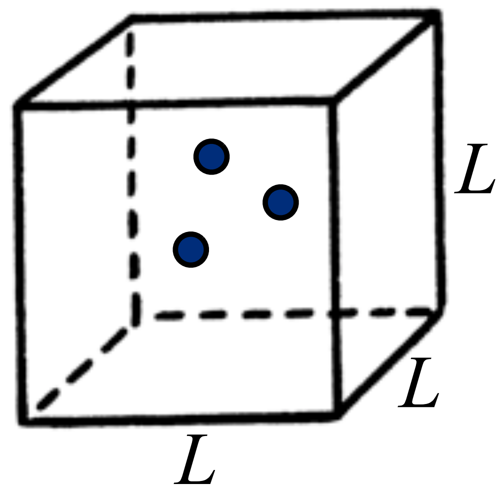
$$E = \frac{6\pi a \pm \sqrt{(6\pi a)^2 + \frac{1}{|r_3|}}}{L^3} + O(L^{-4})$$

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 $(r_3 \to -\infty)$,

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

$$E_2 \approx -\frac{1}{12\pi a|r_3|L^3}$$ (another 3-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

$$E \approx +\frac{1}{|r_3 D|} - i(\text{small imaginary part})$$

Summary

- Determined the special three-body wave functions at a three-body resonance in powers of *1/{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
- ...