Mass dependent energies and scattering lengths for three and four-particle two-component systems under 1D confinement

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Outline of this talk

I. Current experiments with cold atoms

II. Two-Body problem

III. Three-body HHL Problem
   a) The Born-Oppenheimer potential curve
   b) Numerical results and comparison with more accurate methods

IV. Four-body HHHL Problem
   a) The coordinates
   b) The Born-Oppenheimer surface
   c) Numerical results

V. Current & future work
Atoms in waveguides

- Tune the laser frequency a little to the red of an atomic transition
- The “AC Stark shift” results in an effective potential energy well.

Assumption for this work: Atoms remain confined to the lowest transverse mode, and the Olshanii formula is meaningful.

$$a = -\frac{a_{\perp}^2}{2a_{3D}} \left( 1 - C \frac{a_{3D}}{a_{\perp}} \right)$$

$$C \approx 1.4603$$
Low-energy (2-body) scattering in 1D

\[ \psi(x) \rightarrow \begin{cases} 
\sin(kx + \delta) & \text{odd} \\
\cos(kx + \delta) & \text{even}
\end{cases} \]

For \( V(x) = g\delta(x) \),

\[ a = -\frac{1}{(\mu g)} \]

\[ V(x) = \frac{-1}{\mu a} \delta(x) \]

For one heavy (H) and one light (L):

\[ \beta = \frac{m_L}{m_H} \]

\[ \mu_{HL} = m_H \frac{\beta}{1 + \beta} \]

\[ B_2 = \frac{1}{m_H a^2} \frac{\beta + 1}{2\beta} \]
Some questions I want to answer:

- What are the energy levels for the HHL and HHHL system?
- What is the atom-dimer $a_{AD}$ scattering length for H+HL $\rightarrow$ H+HL?
- What is the atom-trimer $a_{AT}$ scattering length for H+HHL $\rightarrow$ H+HHL?
- What are the specific mass ratios at which a new bound state appears (and $a_{AD}$, $a_{AT}$ diverge)?
- What are the specific mass ratios at which $a_{AD}$ or $a_{AT}$ is zero?
Born-Oppenheimer approximation for the 3-body problem

In units of the HL binding energy:

\[
\begin{align*}
[\hat{T}_H + \hat{V}_{HH}]\Psi &= \left\{ \begin{array}{l}
- \frac{1}{2\mu_3} \frac{\partial^2 \Psi}{\partial x^2} + g_3 \lambda \delta(2x_0) \Psi \\
- \frac{1}{2\mu_3} \frac{\partial^2 \Psi}{\partial y^2} + g_3 \left[ \delta(y + x_0) + \delta(y - x_0) \right] \Psi \\
= \hat{H}_{ad} \Psi
\end{array} \right.
\end{align*}
\]

\[
\mu_3 = \frac{1 + \beta}{2\sqrt{\beta(2 + \beta)}}
\]

\[
g_3 = -2\sqrt{2} \left( \frac{\beta}{2 + \beta} \right)^{1/4}
\]

\[
x_0 = x \sqrt{\frac{\beta}{2 + \beta}}
\]

Born-Oppenheimer factorization:

\[
\Psi(x, y) = \Phi(x; y) \psi(x)
\]

\[
\Phi(x; y) = u(x) \Phi(x; y),
\]

\[
\Psi(x, y) = \left( \frac{-1}{2\mu_3} \frac{\partial^2}{\partial x^2} + g_3 \lambda \delta(2x_0) + u(x) + \frac{\tilde{Q}(x)}{2\mu_3} \right) \psi(x) = E \psi(x)
\]

\[
\tilde{Q}(x) = \left\langle \frac{\partial \Phi}{\partial x} \left| \frac{\partial \Phi}{\partial x} \right\rangle_y
\]

Jacobi Coordinates:
3-Body HHL problem

... with this potential for $x$-dependent eigenvalues $u(x)$.

Solve fixed-$x$ Schrödinger equation along this line...

Obtain a transcendental equation for the eigenvalue:

$$\frac{\kappa}{g_3 \mu_3} + 1 = (-1)^{P+1} e^{-2\kappa x_0}.$$
The nonadiabatic correction

\[ \frac{\kappa}{g_3 \mu_3} + 1 = (-1)^{P+1} e^{-2\kappa x_0}. \]

\[ \kappa(x) = \sqrt{-2\mu_3 u(x)} \]

\[ \tilde{Q}(x) = \left< \frac{\partial\Phi}{\partial x} \right| \frac{\partial\Phi}{\partial x} \right> \]

\[ \dot{Q}(x) = \frac{\beta}{3(2 + \beta)} (-2hx_0 + 2\kappa x_0 + 1)^4 \times \left[ 3h^2 + x_0 (-12h^3 + 24h^2 \kappa - 36h^2 \kappa + 24\kappa^3) + x_0^3 (-16h^3 \kappa^2 + 48h^2 \kappa^3 - 48h^2 \kappa^2 + 16\kappa^5) + x_0^2 (12h^4 - 48h^3 \kappa + 108h^2 \kappa^2 - 120h^2 \kappa^3 + 48\kappa^4) + x_0^4 (-16h^4 \kappa^2 + 64h^3 \kappa^3 - 96h^2 \kappa^4 + 64h^2 \kappa^5 - 64\kappa^6) \right], \]

\[ h = \mu_3 g_3 \]

\[ \lim_{|x| \to \infty} u(x) = -1 - \frac{\beta}{2 + \beta} \]

\[ \lim_{|x| \to \infty} \left[ u(x) + \frac{\tilde{Q}}{2\mu_3} \right] = -1 + \left( \frac{\beta}{2 + \beta} \right)^2. \]
Results for the HHL system

For Li-Cs mixtures ($m_H/m_L \approx 22$)

(bosons $\lambda = 0$)

(bosons $\lambda = \infty$, or NI fermions)

These potential curves give the spectrum & $\sigma_{AD}$ for one mass ratio
Comparison with Kartavtsev, Malykh and Sofianos

TABLE I. The values of the mass ratio $\beta^{-1} = m_H/m_L$ for which the atom-dimer scattering length is infinite ($a_{AD} \rightarrow \infty$, corresponding to the appearance of the $n^{th}$ trimer state), or zero ($a_{AD} \rightarrow 0$), are tabulated both the case of noninteracting bosonic H atoms ($\lambda \rightarrow 0$) and fermionic H atoms ($\lambda \rightarrow \infty$). Results are compared to Ref. [23]. An asterisk (*) denotes an exact result.

<table>
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<th>$n$</th>
<th>$\lambda = 0$</th>
<th>$\lambda = 0$</th>
<th>$\lambda = \infty$</th>
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<td>$\beta^{-1}<em>{a</em>{AD} \rightarrow 0}$</td>
<td>$\beta^{-1}<em>{a</em>{AD} \rightarrow \infty}$</td>
<td>$\beta^{-1}<em>{a</em>{AD} \rightarrow 0}$</td>
<td>$\beta^{-1}<em>{a</em>{AD} \rightarrow \infty}$</td>
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<td>214.331</td>
<td>213.964</td>
<td>221.133</td>
<td>220.765</td>
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From KM&S

Heavy particle coordinates make the x-y plane.

Because H-particles are identical, only need $0 < \varphi < \pi / 6$ (for a given parity).

Solve the fixed $(\rho, \varphi)$ Schrodinger equation (along the red line).

Plot the eigenvalue $U(\rho, \varphi)$. 

\[
z \sim \left( \frac{x_1 + x_2 + x_3}{3} - \tilde{\gamma} x_4 \right)
\]

\[
y \sim \left( \frac{x_1 + x_2}{2} - x_3 \right)
\]

\[x \sim x_1 - x_2\]
Where are the interactions?

Heavy particles have a definite ordering within this wedge.

\[ z \sim \left( \frac{x_1 + x_2 + x_3}{3} - \tilde{y} x_4 \right) \]

\[ z \sim \left( \frac{x_1 + x_2}{2} - x_3 \right) \]

\[ x \sim x_1 - x_2 \]

\[ \Phi(\rho, \phi; z) = U(\rho, \phi) \Phi(\rho, \phi; z) \]

\[ \frac{z}{\rho\gamma/\sqrt{2}} \]

\[ \begin{cases} 
- \frac{\rho\gamma}{\sqrt{2}} \sin (\phi + \pi/3) \\
- \frac{\rho\gamma}{\sqrt{2}} \sin (\phi - \pi/3) \\
\frac{\rho\gamma}{\sqrt{2}} \sin (\phi)
\end{cases} \]
The triple delta-function problem

\[ \frac{-\partial^2}{\partial z^2} + g_a \delta(z - a) + g_b \delta(z - b) + g_c \delta(z - c) \right\} \Phi(z) = -\kappa^2 \Phi(z) \]

\[ g_a g_c (g_b - 2\kappa) e^{2\kappa(a+b)} - g_a g_b (g_c + 2\kappa) e^{2\kappa(a+c)} + (g_a + 2\kappa)(g_b + 2\kappa)(g_c + 2\kappa) e^{2\kappa(b+c)} - g_b g_c e^{4b\kappa} (g_a + 2\kappa) = 0 \]

\[ g_a = g_b = g_c = 2\mu_4 g_4, \]

\[ \kappa^2 = -2\mu_4 U(\rho, \phi) > 0, \]

\[ a = z_1, \ b = z_2 \text{ and } c = z_3. \]
HHHL potential energy surface & curves (for $m_H/m_l \approx 22$) (Even parity)

Solve the fixed-$\rho$ equation to get "hyperspherical" curves
The energy landscape \((m_H/m_L \approx 22)\)

![Graphs showing energy landscapes for Bosons and Fermions](image)
The HHL Spectrum and the atom-trimer scattering length $a_{AT}$ (Even Parity)

Bosons

Fermions

\[(m_H/m_L)^{1/2}\]

\[E/B_2\]

\[\tan^{-1}(a_{AT}/a) / \pi\]

\[(m_H/m_L)^{1/2}\]
The HHL Spectrum and the atom-trimer scattering length $a_{AT}$ (Odd Parity)

*preliminary results

Bosons

Fermions
Current and Future Work

- Treat arbitrary heavy particle interactions. (not just the noninteracting, or infinitely repulsive cases.)
- Construct an HHHL “phase diagram”.
- Add harmonic confinement, compare with recent publications.
- Work towards a fully 3D 3-body problem with a cigar-trap?
- Other systems like HLL, HHLL, HLLL?
- Thanks to Jose D’Incao and Jesper Levinson for helpful discussions. Thanks also to C.H. Greene for early inspiration to start this problem.

THANK YOU!