Elastic Collision Phenomena in Quantum Gases

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Where do we stand?

1. We studied dependence of scattering length on well parameter
2. We found resonant enhancement near the bound state threshold
3. We found universal behavior near the threshold
4. We defined halo states and zero-range potentials
5. We analyzed the energy dependence of the scattering length
6. We introduced the effective range $r_e$
7. We discussed anomalously large and small scattering lengths
8. We noticed that negative effective ranges did not appear
9. We found $r_e$ to be important only for anomalously large $a$
Relative motion of interacting particles III

flat-bottom potential

broad s-wave resonances
s-wave resonances

We return to the energy dependence of the phase shift

\[ \eta_{\text{res}}(k) = -kr_0 + \arctan \left( \frac{k}{K_+ \cot K_+ r_0} \right) \]

\[ a(k) = r_0 - \frac{1}{k} \arctan \left( \frac{k}{K_+ \cot K_+ r_0} \right) \]

\[ K_+^2 = k^2 + \kappa_0^2 \]

\[ a_{\text{res}} = a - r_0 \]

"background"  "resonant"
Breit-Wigner line shape

Expand about resonance \( \delta k = k - k_{res} \)

\[
\tan \eta_{res} = \frac{k}{K_+ \cot K_+ r_0} \approx \frac{1}{\delta k \, r_0} = \frac{-(k + k_{res})}{(k + k_{res})(k - k_{res})r_0} \approx \frac{-2k_{res}}{(k^2 - k_{res}^2)r_0} \equiv -\frac{\Gamma/2}{E - E_{res}}
\]

\[
\sin^2 \eta_{res} = \frac{(\Gamma/2)^2}{(E - E_{res})^2 + (\Gamma/2)^2}
\]

\[
\Gamma = \left(\frac{\hbar^2}{m_r}\right)(2k_{res}/r_0)
\]

\[
\sigma_0 = \frac{4\pi}{k^2} \sin^2 \eta_0 \quad \Rightarrow \quad \sigma_0 = \frac{4\pi}{k_{res}^2} \frac{(\Gamma/2)^2}{(E - E_{res})^2 + (\Gamma/2)^2}
\]
s-wave resonance near threshold

\[ a(k) = r_0 - \frac{1}{k} \arctan \frac{k}{K_+ \cot K_+ r_0} \]

\[ a(k) \approx r_0 + \frac{1}{k} \arctan \frac{k}{\kappa} \quad \text{(weakly-bound level)} \]

\[ a(k) \approx r_0 - \frac{1}{k} \arctan \frac{k}{\kappa_{VS}} \quad \text{(virtual level)} \]
s-wave resonance near threshold

\[ a(k) = r_0 - \frac{1}{k} \arctan \left( \frac{k}{K_+ \cot K_+ r_0} \right) \]

Conclusion: scattering length approximation valid for

[Diagram showing the resonance condition and the expression for \( a(k) \).]

\[ k \ll \kappa \ll \kappa_{vs} \]
from halo state to narrow resonance

Bound states ($\varepsilon < 0$):

$$\chi_0 = Ae^{-\kappa r}$$

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'open' channel

\begin{align*}
K_{-r_0} &= (v_{\text{max}} + \frac{1}{2})\pi \\
K_{-r_0} &= \pi \\
K_{-r_0}^2 &= \kappa_0^2
\end{align*}

'closed' channel

\begin{align*}
K_{+r_0} &= v\pi \\
K_{-r_0} &= v\pi \\
\kappa_1 \delta(r - r_0)
\end{align*}
screened flat-bottom potential

narrow s-wave resonances
screened flat-bottom potential

\[ r > r_0 \quad U_0(r) = 0 \quad \chi_0'' + k^2 \chi_0 = 0 \]
\[ \chi_0 = A \sin(kr + \eta_0) \]
\[ \chi_0' = kA \cos(kr + \eta_0) \]

\[ r < r_0 \quad U_0(r) = -\kappa_0^2 \quad \chi_0'' + K_+^2 \chi_0 = 0 \]
\[ \chi_0 = A' \sin(K_+r + \eta_0') \]
\[ \chi_0' = K_+A' \cos(K_+r) \]

boundary condition: \( \chi_0(r) \) continuous, \( \chi_0'(r) \) jumps at \( r = r_0 \)

\[ \chi_0'/\chi_0|_{r=r_0} = K_+ \cot K_+r_0 = k \cot(kr_0 + \eta_0) + \kappa_1 \]

Barrier parameter: \( \beta \equiv \kappa_1 r_0 \)

\[ a(k) = r_0 - \frac{1}{k} \arctan \left( \frac{kr_0}{K_+r_0 \cot K_+r_0 - \beta} \right) \]
screened flat-bottom potential

Expand about resonance \((\delta k = k - k_{\text{res}})\)

\[
\tan \eta_{\text{res}} = \frac{k}{K_+ \cot K_+ r_0 - \kappa_1} \sim -\frac{1}{\delta k r_0} \frac{\kappa_1^2}{\kappa_0^2} = \frac{-(k + k_{\text{res}})}{(k^2 - k_{\text{res}}^2) r_0} \frac{\kappa_1^2}{\kappa_0^2} \sim \frac{-\Gamma/2}{E - E_{\text{res}}}
\]

\[
\sin^2 \eta_{\text{res}} = \frac{(\Gamma/2)^2}{(E - E_{\text{res}})^2 + (\Gamma/2)^2}
\]

\[
\Gamma = \left(\frac{\hbar^2}{m_r}\right) \left(\frac{2k_{\text{res}}}{R^*}\right)
\]

\[
R^* = \frac{1}{2} r_0 \left(\frac{\kappa_1}{\kappa_0}\right)^2
\]
We analyze the energy dependence of a resonance near threshold.

\[ \eta_0(k) = -kr_0 + \arctan \left( \frac{kr_0}{K_+r_0 \cot K_+r_0 - \beta} \right) \]

“regular” \hspace{1cm} “resonant”

evaluate phase shift:

\[
k \cot \eta_0 = \frac{(K_+ \cot K_+r_0 - \kappa_1) + k^2 r_0 + \cdots}{1 - r_0 \left(1 + \frac{1}{3} k^2 r_0^2 + \cdots \right) (K_+ \cot K_+r_0 - \kappa_1)}
\]

\[ K_+^2 = k^2 + \kappa_0^2 \quad \rightarrow \quad K_+r_0 = \kappa_0 r_0 \left[1 + \frac{k^2}{\kappa_0^2}\right]^{1/2} = \gamma + \frac{1}{2} k^2 r_0^2 / \gamma + \cdots \]

\[ a = r_0 \left(1 - \tan \gamma / \gamma \right) \]
Effective range expansion: $r_e$ : measure for energy dependence of the phase shift

\[ k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2} k^2 r_e + \cdots \]

effective range: $r_e = r_0 \left(1 - \frac{3ar_0 + \gamma^2 r_0^2 - 3\beta(a^2 - r_0^2)}{3a^2\gamma^2} + 3\beta^2(a - r_0)^2}{3a^2\gamma^2} \right)$

broad resonance – open channel ($r_e > 0$ for large $|a|$):

\[ \kappa_1 \to 0 \quad \Rightarrow \quad r_e \simeq r_0 \left(1 - \frac{3ar_0 + \gamma^2 r_0^2}{3a^2\gamma^2}\right) = r_0 \left(1 - \frac{r_0}{a\gamma^2} - \frac{r_0^2}{3a^2}\right) \]

narrow resonance – closed ($r_e < 0$ for large $|a|$):

\[ \kappa_1^2 \gg \kappa_0^2 \quad \Rightarrow \quad r_e \simeq -r_0 \kappa_2 \frac{(a - r_0)^2}{a^2} = -r_0 \kappa_2 \left(1 - 2\frac{r_0}{a} + \frac{r_0^2}{a^2}\right) \]
Resonance-width parameter $R^*$

\[ k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2} k^2 r_e + \cdots \]

narrow resonance – ‘closed’ channel ($r_e < 0$ for large $|a|$):

\[ \kappa_1^2 \gg \kappa_0^2 \quad \rightarrow \quad r_e \simeq -r_0 \frac{\kappa_1^2}{\kappa_0^2} \left(1 - 2 \frac{r_0}{a} + \frac{r_0^2}{a^2}\right) \simeq -2R^* \]

positive

\[ R^* = -\frac{1}{2} r_e \simeq \frac{1}{2} r_0 \left(\frac{\kappa_1}{\kappa_0}\right)^2 \]

strong barrier – weak coupling – narrow resonance – closed channel $R^* \gg r_0$

weak barrier – strong coupling – broad resonance – open channel $R^* \ll r_0$
narrow resonance near threshold

\[ a = \frac{1}{\kappa} \]

\[ a > 0 \]

\[ a < 0 \]

\[ a = -\frac{1}{\kappa_{qb}} \]

\[ -\kappa_0^2 \]

\[ + \varepsilon_{qb} \]

\[ - \kappa^2 \]

\[ + \varepsilon_{qb} \]

\[ - \kappa^2 \]

\[ - \kappa_0^2 \]

\[ \frac{a(k)}{r_0} \]

\[ k r_0 \]

\[ a(k) = r_0 - \frac{1}{k} \arctan \left( \frac{k r_0}{K_+ r_0 \cot K_+ r_0 - \beta} \right) \]

\[ K_+^2 = k^2 + \kappa_0^2 \]
particles with internal structure
(scattering of atoms)
Schrödinger equation

\[ \left( \frac{1}{2\mu} \left( p_r^2 + \frac{L_z^2}{r^2} \right) + V(r) \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi) \]

thus far: fixed potential

What happens if we add internal structure?

First we recapitulate:

\( L_z, L_z \) commute with \( r \) and \( p_r \)

separation of variables:

\[ \psi = R_l(r)Y^m_l(\theta, \phi) \]

\[ L^2 Y^m_l(\theta, \phi) = l(l+1)\hbar^2 Y^m_l(\theta, \phi) \]

\[ L_z Y^m_l(\theta, \phi) = m\hbar Y^m_l(\theta, \phi). \]

\[ \left( \frac{\hbar^2}{2\mu} \left( -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} \right) + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) \right) R_l(r) = E R_l(r) \]

\[ V_{\text{eff}}(r) \]

good for systems like helium
Interactions between alkali atoms

For two ground-state alkali atoms, two (not more than two) potentials

\[
V_S(r) = \begin{cases} 
V_1(r) & S = 1 \\
V_0(r) & S = 0 
\end{cases}
\]

Conclusion: exchange determines interatomic interaction

To solve Schrödinger equation, we turn to the basis:

\[
|\psi\rangle = |R_l\rangle |lm_l; \psi_e\rangle |S, M_S\rangle
\]
Interactions between alkali atoms

To represent exchange we construct a spin hamiltonian:

\[ V(r) = V_D(r) + J(r)s_1 \cdot s_2 \]

\[ J(r) = V_1(r) - V_0(r) \]

\[ V_D(r) = \frac{1}{4}[V_0(r) + 3V_1(r)] \]

Properties of operator \( V(r) \):

\[ V(r) |0, 0\rangle = V_0(r) |0, 0\rangle \]

\[ V(r) |1, M_S\rangle = V_1(r) |1, M_S\rangle \]

Hamiltonian including exchange:

\[ \mathcal{H} = \frac{1}{2\mu} \left( p_r^2 + \frac{L^2}{r^2} \right) + V(r) \]
Interactions between alkali atoms

Let us add magnetic field:

$$\mathcal{H}_Z = \gamma_e s_1 \cdot B + \gamma_e s_2 \cdot B = \gamma_e S \cdot B = \gamma_e B S_z$$

$$\gamma_e = g_s \mu_B / \hbar$$

$$\Delta E_Z = g_s \mu_B B M_S$$

$$M_S = m_{s_1} + m_{s_2}$$ is good quantum number

$$s_1 \cdot s_2 = \frac{1}{2} (S^2 - s_1^2 - s_2^2)$$

$$s_1 \cdot s_2 = s_{1z}s_{2z} + \frac{1}{2} (s_1^+s_2^- + s_1^-s_2^+)$$

Hamiltonian including spin Zeeman term:

$$\mathcal{H} = \frac{1}{2\mu} \left( p_r^2 + \frac{L^2}{r^2} \right) + V(r) + \gamma_e B S_z$$

good basis states: $$|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle$$
Interactions between alkali atoms

Hamiltonian including spin Zeeman term:

\[ H = \frac{1}{2\mu} \left( p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + V(r) + \gamma_e B S_z \]

good basis states: \[ |\psi\rangle = |R_{v,l}^S\rangle |S, M_S\rangle |l, m_l\rangle \]

Solve radial wave equation for given \( l, S \) and \( M_S \):

\[ R''_{S,l} + \frac{2}{r} R'_{S,l} + \left[ \varepsilon - U_{S,l}(r) \right] R_{S,l} = 0 \]

\[ U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} \gamma_e B M_S \]
Interactions between alkali atoms

The magnetic field lifts the degeneracy of the triplet potential, making it possible to shift the triplet potential with respect to the singlet potential.

\[ U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} \gamma e B M_S \]

This makes it possible to shift the triplet potential with respect to the singlet potential.
Feshbach resonance

We can vary the collision energy to be resonant with a bound state in a closed channel.

Any weak singlet-triplet coupling induces a scattering resonance in the open channel: Feshbach resonance.

With cold alkali atoms we can tune to a Feshbach resonance at arbitrary, fixed (low) collisional energy by varying the magnetic field: Zeeman tuning.
some nomenclature

Closed channel: below threshold

\[ \varepsilon_v = -\kappa^2 \]

Closed channel: above threshold

\[ a > 0 \]

threshold energy

\[ \varepsilon_{qb} \]

\[ \varepsilon_{qb} \]

\[ \varepsilon \]

\[ 0 \]

\[ \varepsilon_{v} = -\kappa^2 \]

\[ \kappa^2 \]

\[ \kappa^2 \]

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particles with internal structure

1. We analyzed s-wave resonances
2. We noticed that negative effective ranges did not appear
3. We introduced a tunnel barrier
4. We found that for a weak tunnel coupling $r_e < 0$
5. We introduced the width parameter $R^*$ to discriminate between broad and narrow s-wave resonances
6. We introduced atoms with spin
7. We found triplet and singlet potentials
8. We introduced the Feshbach problem