Physics 471 – Introduction to Modern Atomic Physics

HOMEWORK 4 (Due: 2/10/2024)

1. Potential resonance and Fermi pseudo-potential

Interactions between neutral atoms are described by a short-range molecular potential $V(\vec{r})$. The potential quickly drops to zero when interatomic separation r exceeds the range of the potential r_0. Here we assume $V(r > r_0) \approx 0$. At short range $r < r_0$, the potential can be attractive and very complex, and it may support many molecular bound states.

In the relative coordinate the Hamiltonian $H = \frac{p^2}{2\mu} + V(R)$, where $\mu = m_1 m_2/(m_1 + m_2)$ is the reduced mass. An incident *s*-wave $\psi_{in}(R) = e^{ikR}/R$ is scattered by the potential and results in an outgoing wave $\psi_{out}(r > r_0) = -Se^{-ikr}/r$, where $S = e^{2i\delta}$ is the s-wave scattering matrix and δ is the scattering phase shift.

For no interaction, the solution of the Schroedinger's equation is $\psi = \psi_{in} + \psi_{out} \propto \frac{\sin kr}{r}$ and thus scattering phase shift $\delta = 0$.

A. Scattering length a is defined as the position where the scattering wavefunction is expected to vanish in the zero scattering energy limit $\lim_{k \to 0} \psi(r > r_0) \propto 1 - \frac{a}{r}$. Show that this definition is equivalent to the formal definition of the scattering length, given by

$$\lim_{k \to 0} k \cot \delta = \frac{(r\psi)'}{r\psi} = -\frac{1}{a}$$

B. A new molecular bound state emerges at the continuum with energy $E = -E_b = 0$, when scattering length diverges $a \to \pm\infty$. Here E_b is the molecular binding energy. The divergence happens when $\delta = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}$ ... To prove this, show that when the scattering length diverges on the positive side $a \to +\infty$, a bound state exists with vanishing binding energy $E_b = \frac{\hbar^2}{2\mu a^2}$.

C. When the interaction range is small compared to all relevant length scale $r_0 \approx 0$, we may introduce the *Fermi pseudo-potential* $V_{eff}(r) = \frac{2\pi\hbar^2 a}{\mu}\delta(r)$, which can fully describe the physics of low energy scattering with the original molecular potential $V(r)$.

Hint: Assume $\psi(r) \propto 1 - \frac{a}{r}$ is valid for all $r > 0$ and is the eigenstate of the Hamiltonian $H = \frac{p^2}{2\mu} + V_{eff}(r)$ with a vanishing eigenenergy $E = 0$.

D. Show that the pseudo potential $V_{eff}(r)$ supports a single bound state when $a > 0$ and determine the wavefunction of the molecular bound state.

2. Feshbach resonance

Feshbach resonances in collisions of cold atoms occur when two atoms in an open channel collide and couple to a molecular state in a closed channel. Here a channel refers to the internal state of the atoms or molecules. When the total energy of the system is above (below) the dissociation energy of the channel, the channel is considered open (closed)

Consider the system can be prepared in the open channel ψ_o and closed channel ψ_c. The wavefunction is given by $\psi(r) = \begin{pmatrix}\psi_c(r)\\ \psi_o(r)\end{pmatrix}$, and the Hamiltonian is $H = \frac{p^2}{2\mu}\hat{1} + \hat{V}(r)$. Here $\hat{1}$ is identity matrix and $\hat{V}(r)$ is the spin-dependent molecular potential. We assume the closed channel is inaccessible outside the interaction range $\hat{V}(r > r_0) = \begin{pmatrix}\infty & 0\\ 0 & 0\end{pmatrix}$ and the short-range potential is attractive $\hat{V}(r < r_0) = -\begin{pmatrix}V_c & \varepsilon\\ \varepsilon & V_o\end{pmatrix}$, where ε couples the open and closed channels.

A. We initially prepare free atoms in the open channel with low energy $E = \frac{\hbar^2 k^2}{2\mu} \ll V_c, V_o$. After scattering the s-wave wavefunction is phase shifted as $r\psi(r > r_0) = \begin{pmatrix}0\\ \sin(kr + \delta)\end{pmatrix}$. Show that

$$k\cot(kr_0 + \delta) = q_+ \cos^2\alpha \cot q_+ r_o + q_- \sin^2\alpha \cot q_- r_0, \qquad (1)$$

where $\tan 2\alpha = \frac{2\varepsilon}{V_c - V_0}$ and $\hbar^2 q_\pm^2/2\mu$ are the eigen-energies at short range. In the limit of zero coupling $\varepsilon \to 0$ the eigen-energies approach V_o and V_c, respectively.

Hint: Use the continuity of the wavefunction $\psi(r_0^+) = \psi(r_0^-)$ and $\psi'(r_0^+) = \psi'(r_0^-)$.

Remark: In atoms, weak coupling $\varepsilon << |V_C - V_o|$ is a very good approximation since spin-spin interactions (typically GHz) is very weak compared to exchange interactions (typically 100THz).

B. We may assume that the closed channel supports a bound state at energy $E = E_c$ close to the open channel threshold $E = 0$. Show that the 2[nd] term contributes to the phase shift resonantly as

$$k\cot(kr_0 + \delta) = q_+ \cos^2\alpha \cot q_+ r_0 - \frac{\Gamma/2}{r_0 E_c},$$

where we have define the Feshbach coupling strength as $\Gamma \approx 4\alpha^2 V_c$.

Hint: The existence of the bound state in the square potential suggests $\sin\sqrt{\frac{2\mu}{\hbar^2}(V_c + E_c)}r_0 = 0$. Since the bound state is near the continuum, we can assume $|E_c| \ll V_c$

C. Show that the scattering length is linked to boundary conditions $\lim_{k\to 0} k\cot(kr_0 + \delta) = -\frac{1}{a - r_0}$ in the low energy limit, and we can rewrite $q_+ \cos^2\alpha \cot q_+ r_0 = -\frac{1}{a_{bg} - r_0}$, where a_{bg} is the background scattering length far from the resonance $\Gamma/2r_0 E_c \to 0$.

D. Experimentally, the bound state energy is magnetically tuned as $E_c = \mu(B - B_c)$, where μ is the magnetic moment of the molecular state and B_c is the field that the state crosses the continuum. Show that we arrive at the universal expression of scattering length across a Feshbach resonance.

$$a = a_{bg}(1 - \frac{\Delta B}{B - B_0}).$$

Determine the resonance width ΔB and resonance position B_0 in terms of a_{bg}, Γ, μ and B_c.