Confinement induced resonance

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We present a formal derivation of the confinement induced resonance for particles in a lower dimension. The generic T-matrix method is used to calculate the S-wave collisional property between two ultra-code atoms. We show the breakdown of a naive approach to describe such low dimensional system near a Feshbach resonance and preform a real three dimensional calculation to include additional effect from the confinement. The normalization of the high energy states in such cases are done by comparing to the result in free space.

1. INTRODUCTION

In the field of ultra-cold atoms and molecules, the collisional properties between the particles play an important role for cooling into quantum degeneracy. The tunability of the scattering length using Feshbach resonance opens the door for engineering the interaction and using it as a source of correlation and entanglement in a many-body system.

2. SCATTERING THEORY

In this section, we will describe a formal way to calculate the properties of S-wave scattering between two atoms at low temperature.

2.1. Wave function of a scattering process

In a scattering problem, the wave function can be broken into the incident wave Ψ_i and the scattered wave Ψ_s where the incident wave is usually a plain wave

$$\Psi_i = e^{i\vec{k}\cdot\vec{r}}$$

and the scattered wave can be expressed as a spherical wave centered around the scattering core ($\vec{r} = 0$)

$$\Psi_s = \frac{f(\theta)}{r}e^{ik'r}$$

For all the discussion in this paper, we are taking the limit of low temperature (i.e. low kinetic energy) in which case the scattering is limitted to S-wave (angular momentum $L^2 = 0$). We also assume that the interaction is short range so that the behavior is regular for long wavelength and we can take the limit of $k \to 0$. In such a limit, the total wave function can be written as

$$\Psi(\vec{r}) = \Psi_i(\vec{r}) + \Psi_s(\vec{r})$$
$$\approx e^{i\vec{k}_0\cdot\vec{r}} - \frac{a}{r}$$

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where a, which describe the fraction being scattered, is defined as the scattering length. In order to solve this problem, it is convinient to express the Schrödinger equation in the momentum space

$$\frac{k^2 - k'^2}{m}\Psi_s\left(\vec{k}'\right) = U\left(\vec{k}',\vec{k}\right) + \int \frac{\mathrm{d}^3 k''}{(2\pi)^3}U\left(\vec{k}',\vec{k}''\right)\Psi_s\left(\vec{k}''\right)$$

where $U\left(\vec{k}',\vec{k}\right)$ is the Fourier transform of the interaction

$$U(\vec{k}',\vec{k}) = \int \mathrm{d}^3\vec{r} \int \mathrm{d}^3\vec{r}' U(\vec{r}' - \vec{r})e^{i\vec{k}'\cdot\vec{r}'}e^{-i\vec{k}\cdot\vec{r}}$$

and we have used the fact that the interaction is short range and the energy of the state is determined by the long distance behavior of the incident state $E_k = k^2/2m$.

2.2. T-Matrix

The T-matrix is defined as a map from the initial state of the scattering (which is a δ function in k space in our case) to the final state. It is defined as,

$$\hat{T} = \hat{V} + \hat{V}\frac{1}{E - \hat{H}_0 + i0}\hat{T}$$

For the scattering process in free space, the equation above can be represented in k space as,

$$T\left(\vec{k}',\vec{k},E\right) = U\left(\vec{k}',\vec{k}\right) + \int \frac{\mathrm{d}^3 k''}{(2\pi)^3}\frac{U\left(\vec{k}',\vec{k}''\right)}{E - k''^2/m + i0}T\left(\vec{k}'',\vec{k},E\right)$$

where the $+i0$ denotes a infinitesimal quantity to ensure that we have outgoing waves. Note the similarity with the equation satisfied by the scattered wavefunction. Using the T-matrix, we can express the scattered wavefunction as

$$\Psi_s\left(\vec{k}'\right) = \frac{m}{k^2 - k'^2 + i0}T\left(\vec{k}',\vec{k},\frac{k^2}{m}\right)$$

And we cans also define the scattering amplitude as

$$f\left(\vec{k}',\vec{k}\right) = -\frac{m}{4\pi}T\left(\vec{k}',\vec{k},\frac{k^2}{m}\right)$$

For the problem we are considering, we will take the limit of $k, k' \to 0$, therefore

$$\Psi_s\left(\vec{k}'\right) = \frac{m}{k^2 - k'^2 + \mathrm{i}0} T(0,0,0)$$

In real space

$$\Psi_s(\vec{r}) = \int \frac{\mathrm{d}k'^3}{(2\pi)^3} \frac{m \mathrm{e}^{\mathrm{i}\vec{k}'\cdot\vec{r}}}{k^2 - k'^2 + \mathrm{i}0} T(0,0,0)$$
$$= -\frac{m \mathrm{e}^{\mathrm{i}kr}}{4\pi r} T(0,0,0)$$

and by comparing to the form of Ψ_s at low temperature we have $f(k \to 0) = -a$

2.3. Effective interaction

Althought the interaction potential between two atoms can be very strong and hard to calculate, they are usually very short range and their precise behavior can only affect the states with a large k. Therefore, for the purpose of low energy collision in which both the initial and final state has a small k, it is useful to introduce a simple effective potential that can be used to describe these low energy process below a cut-off energy ε_c. Let the corresponding cut-off in wave vector and length be $k_c^2/m = \varepsilon_c$ and $R_c = k_c^{-1}$, we can write a effective potential $\tilde{U}\left(\vec{k}', \vec{k}\right)$

$$\tilde{U}\left(\vec{k}', \vec{k}\right) = U\left(\vec{k}', \vec{k}\right) + m \int_{k_c} \frac{\mathrm{d}^3 k''}{(2\pi)^3} \frac{U\left(\vec{k}', \vec{k}''\right)}{k^2 - k''^2 + \mathrm{i}0} \tilde{U}\left(\vec{k}'', \vec{k}\right)$$

And express the scattering process using this potential and only low energy states as

$$T\left(\vec{k}', \vec{k}, E\right) = \tilde{U}\left(\vec{k}', \vec{k}\right)$$
$$+ \int^{k_c} \frac{\mathrm{d}^3 k'}{(2\pi)^3} \frac{\tilde{U}\left(\vec{k}', \vec{k}''\right)}{E - k''^2/m + \mathrm{i}0} T\left(\vec{k}'', \vec{k}, E\right)$$

The effective potential can now be any short range function that gives the correct scattering amplitude. As the simplest potential, the one that is usually taken is a δ function

$$U(\vec{r}) = U_0 \delta^3(\vec{r})$$

Using which we can write the equation for the scattering amplitude

$$f\left(\vec{k}', \vec{k}\right) = -\frac{mU\left(\vec{k}' - \vec{k}\right)}{4\pi}$$
$$+ m \int^{k_c} \frac{\mathrm{d}^3 k''}{(2\pi)^3} \frac{U\left(\vec{k}' - \vec{k}''\right) f\left(\vec{k}'', \vec{k}\right)}{k^2 - k''^2 + \mathrm{i}0}$$

Since the major contribution of the integral comes from when $|k| = |k''|$, we can replace $f\left(\vec{k}'', \vec{k}\right)$ by $f(k)$ therefore

$$\frac{1}{f(k)} = -\frac{4\pi}{mU_0} + 4\pi \int^{k_c} \frac{\mathrm{d}^3 k''}{(2\pi)^3} \frac{1}{k^2 - k''^2 + \mathrm{i}0}$$
$$= -\frac{4\pi}{mU_0} + \frac{2}{\pi} \left(-k_c - \frac{k}{2} \ln\left(-\frac{k_c - k - \mathrm{i}0}{k_c + k + \mathrm{i}0} \right) \right)$$
$$\approx -\frac{4\pi}{mU_0} + \frac{2}{\pi} \left(-k_c - \frac{\mathrm{i}\pi k}{2} + \frac{k^2}{k_c} \right)$$

therefore

$$a = \frac{\pi}{2} \frac{mU_0}{mU_0 k_c + 2\pi^2}$$

Note that non of the cut-off k_c or the effective potential U_0 is physical but the scattering length a is. Any physical process calculated with the effective model should only depend on physical quantities and k_c and U_0 should drop out.

3. CONFINEMENT INDUCED RESONANCE

When atoms are confined in a strong trapping potential in certain directions but not in the others, their motion in the confined directions can be completely frozen out if the chemical potential of each partical is much smaller than the excitation energy of the trap. On the other hand, in the other directions, there is no trapping potentials and the motion of the atoms are effectively the same with that of atoms in a lower dimension. When considering the collisional properties in such a geometry, one might naively expect that the confinement does not contribute much because of the difference in energy scales. This assumption is usually true but can break down near a Feshbach resonance. Due to the strong interaction between the atoms, high vibrational state in the confined direction can be virtually excited during a collision and therefore modify the properties of the collision.

The right way to study the process is to do a three dimensional calculation of the collision which include all the transversely excited states. In this section, we will use the framework we have developed above to calculate the collisional properties in a strong harmonic transverse potential. In order to normalize the result at the cut-off energy scale, we compare our result to the well-known free-space Feshbach resonance.

3.1. Separation of motion

The advantage of using harmonic confinement is that center-of-mass (COM) motion and the relative motion

can be separated. Given the Hamiltonian of two interacting particles

$$H = \frac{1}{2m} \sum_{i;\alpha} p_{i\alpha}^2 + \frac{m\omega^2}{2} \sum_{i;\alpha < d_\perp} x_{i\alpha}^2 + U$$

where $i = 1, 2$ is the index of particles, α is the index of dimensions, $d_\perp$ is the number of confined dimensions and $U = U(\vec{r}_1, \vec{r}_2)$ is the interaction potential. If we define center-of-mass coordinates

$$X_\alpha = \frac{x_{1\alpha} + x_{2\alpha}}{2} \qquad P_\alpha = p_{1\alpha} + p_{2\alpha}$$

and relative coordinates

$$x_\alpha = x_{1\alpha} - x_{2\alpha} \qquad p_\alpha = \frac{p_{1\alpha} - p_{2\alpha}}{2}$$

the new coordinates still satisfies the canonical commutation relation and the Hamiltonian is fully separated

$$H = H_{CM} + H_{rel}$$
$$H_{CM} = \frac{1}{4m} \sum_\alpha P_\alpha^2 + m\omega^2 \sum_\alpha X_\alpha^2$$
$$H_{rel} = \frac{1}{m} \sum_\alpha p_\alpha^2 + \frac{m\omega^2}{4} \sum_\alpha x_\alpha^2 + U(\vec{r}_{12})$$

And the relative motion problem, therefore the collision problem, is reduced to a single partical problem.

3.2. Calculation of the T-matrix

Instead of the k bases we used for the free-space problem, it is convinient to use the eigen-functions of the non-interacting Hamiltonian as our basis.

$$\phi = \prod_{\beta < d_\perp} \phi_n(x_\beta) \prod_{\alpha \geqslant d_\perp} e^{ik_\alpha}$$

Since we assume only the lowest transverse vibrational state is populated, the quantity we need to calculate is

$$T_{0,0} = \langle 0 | \hat{T} | 0 \rangle$$

where $|0\rangle$ is the ground state of the non-interacting system. Using $\langle r | U | r' \rangle = U_0 \delta(r) \delta(r')$ we have

$$T_{0,0} = U_0 + U_0 T_0 \langle 0 | \frac{1}{E - H_0 + i0} | 0 \rangle$$
$$T_{0,0}^{-1} = U_0^{-1} - \int_0^\infty \langle 0 | e^{(E - H_0 + i0)\tau} | 0 \rangle d\tau$$
$$= U_0^{-1}$$
$$- \int_0^\infty e^{(E+i0)\tau} \left(\frac{m\omega}{4\pi \sinh \omega\tau}\right)^{d_\perp/2} \left(\frac{m}{4\pi\tau}\right)^{(3-d_\perp)/2} d\tau$$

Instead of choosing a cut-off energy scale in order to calculate the integral we can compare this expression to the

result without confinement. Since we know that in the free space $d_\perp = 0$ and when $E = 0$,

$$\frac{m}{4\pi a} = U_0^{-1} - \int_0^\infty \left(\frac{m}{4\pi\tau}\right)^{3/2} d\tau$$

where a is the three dimensional scattering length we replaced the U_0 that needs a cut-off with the integral above and the expression for the T-matrix is

$$T_{0,0}^{-1} = \frac{m}{4\pi a}$$
$$+ \int_0^\infty \left(\left(\frac{m\omega}{4\pi \sinh \omega\tau}\right)^{d_\perp/2} \left(\frac{m}{4\pi\tau}\right)^{(3-d_\perp)/2}\right.$$
$$\left. - \left(\frac{m}{4\pi\tau}\right)^{3/2}\right) e^{(E+i0)\tau} d\tau$$

3.3. Bound state in one dimension

In the case of a one dimentional system, $d_\perp = 2$. Let $\varepsilon = \frac{E}{\omega} - 1$, which is the energy of the system above the zero point energy of the confinement. For low energy state (i.e. $|\varepsilon| \ll 1$)

$$T^{-1} \approx \frac{m}{4\pi a} + \frac{m}{4\pi} \sqrt{\frac{m\omega}{2}} \left(\sqrt{\frac{2}{-\varepsilon}} + O(1)\right)$$

The pole of the T-matrix gives the energy of the bound state and we can see that the energy for the bound states is given by

$$\varepsilon = -m\omega^2 a^2$$

Compare to the case of a free space Feshbach resonance which only have bound states for a positive scattering length, a bound state exist even for negetive scattering length when the system is confined in one dimension.

4. CONCLUSION