Scattering theory for ultracold atoms

Topics of this talk

- Motivation: why do we need a scattering theory for **ultracold atoms**?
  - Physics of the interaction of a quantum gas.
- Recap of fundamentals of two-body scattering theory.
  - Basic definitions.
  - Low-energy scattering, scattering length.
  - Scattering of identical particles.
- Measurement of the interaction properties of quantum gases, universality.
- More concepts from scattering theory
  - Partial wave expansion.
  - T-matrix formalism and Lippman-Schwinger equation.
  - Effective potentials.
- Effective field theory using effective range correction.
  - Modified Gross-Pitaevskii equation.
  - On-shell approximation.
- Multi-channel scattering
  - Open, closed channels.
  - Feshbach resonances.

Interactions in a quantum gases

- In cold atomic gases the interparticle spacing is typically in the order of $\sim 10^2$ nm, an order of magnitude larger than length scale of the interaction.
- It follows that **two body** interactions dominate with respect to three and higher number of particles interaction.
- Moreover, the atoms have a rich hyperfine structure. In a general scattering process, we have the quantum numbers (may refer to spin, atomic species, state of excitation) of the incoming and outgoing states, that may be different. A possible choice of quanutum numbers is called a **channel**.
- At typical temperatures for Bose-Einstein condensation, atoms are at the electronic ground state, so the only relevant degree of freedom is represented by the hyperfine states. The change of states may induce trap loss.
- It is not in general possible to make very precise theoretical calculation for the shape of the potentials, so an interplay of measurements and **effective** theories.

Typical model potentials have the shape

$$V(r) = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}}$$

estimates on the coefficients can be derived using van der Waals model for the interaction.

Recap of basic theory of two-body scattering

Two-body problem I

Let us consider a three-dimensional motion of two distinguishable particles of the same mass m in a unitary volume, in presence of an interaction potential depending only on the distance between the particles. We consider a scattering event in which the *internal degrees of freedom play no role*. This is called a **single-channel** scattering. The relative motion is described by

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where $\hat{H}_0 = \hat{\mathbf{p}}^2/(2m_r)$, $m_r = m/2$ reduced mass. We have a scattered wavefunction expressed as

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \psi_{sc}(\mathbf{r}), \qquad (1)$$

at large distances, the scattered wave is a spherical wave in the form

$$\psi_{sc}(\mathbf{r}) \approx f(\theta, k)\frac{e^{ikr}}{r},$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{r}'$, and k the magnitude of $\mathbf{k}$. The function f is called scattering amplitude. The scattering is elastic, and its energy is

$$E = \frac{\hbar^2 k^2}{2m_r}.$$

The simplest definition of the **scattering length** a is obtained taking the limit of the wavefunction for $k \to 0$. Moreover, the dependence of $f(\theta, k)$ on θ will be throught the function $\cos(\theta)$ for axial symmetry. In this limit the wavefunction is isotropic, so we expect to have a constant $f(\theta) =: -a$,

$$\psi(\mathbf{r}) \approx 1 - \frac{a}{r}. \tag{2}$$

The ratio of the scattered *current of probability* per unit solid angle to the incoming wave current of probability per unit area is the *differential cross section*, which in the case of a incoming plane wave is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\theta, k)|^2,$$

integrating over the whole solid angle we get the total cross section. In the limit of $k \to 0$, we have

$$\sigma = 4\pi a^2.$$

Scattering of identical particles

In the case of identical particles it is necessary to have symmetric or antisymmetric total wavefunctions with respect to the exchange of the particles. Let $\mathbf{k}$ be aligned with the z axis. Then the total wavefunction state reads

$$\psi(\mathbf{r}) = e^{ikz} + f(\theta, k)\frac{e^{ikr}}{r}. \tag{3}$$

Exchanging the particles is equivalent to change the system of reference such that

$$z \to -z, \tag{4}$$

$$\theta \to \pi - \theta, \tag{5}$$

so symmetrized/antisymmetrized wavefunction is

$$\psi(\mathbf{r}) = e^{ikz} + \zeta e^{-ikz} + [f(\theta, k) + \zeta f(\pi - \theta, k)]\frac{e^{ikr}}{r}, \tag{6}$$

where $\zeta = 1$ for bosons, $\zeta = -1$ for fermions. The corresponding cross section gets modified accordingly:

$$\sigma = 8\pi a^2, \tag{7}$$

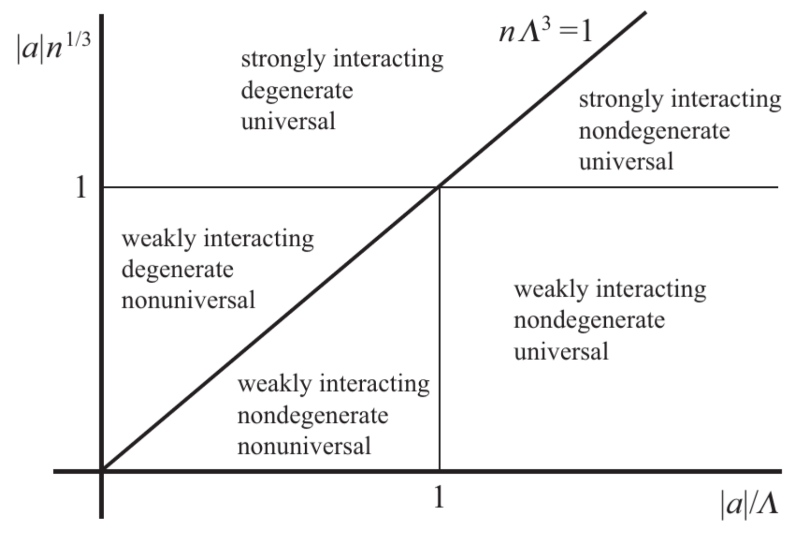
for bosons, $\sigma = 0$ for Fermions.

Measurement of scattering parameters I

In order to measure the scattering parameters, experiments employ the following techniques

- Indirect measure of collision cross-section:
  Working above T_C, in a semiclassical framework, use kinetic theory of gas to relate damping of oscillations to scattering cross section - *require knowledge of particle density*.
- Photoassociation spectroscopy:
  Measures the rate at which two interacting ground-state atoms in an unbound state are excited by means of a laser to a molecular state in which one of the atoms is in a P state.

Measurement of scattering parameters II



More concepts from scattering theory

Partial wave expansion I

The wavefunction can be expanded in *partial waves*

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} A_l P_l(\cos(\theta)) R_{kl}(r), \tag{8}$$

where $R_{kl}(r)$ solves the radial Schrödinger equation

$$R''_{kl}(r) + \frac{2}{r} R'_{kl}(r) + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} V(r) \right] R_{kl}(r) = 0, \tag{9}$$

the asymptotic solution reads

$$R_{kl} \sim \frac{1}{kr} \sin\left(kr - \frac{\pi}{2} l + \delta_l \right) \qquad \text{for} \quad r \to \infty, \tag{10}$$

where δ_l is the l-wave phase shift. Using orthogonality of Legendre polynomials, a similar decomposition is obtained for the scattering amplitude:

$$f(\theta, k) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{i2\delta_l} - 1) P_l(\cos\theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos(\theta)), \tag{11}$$

Partial wave expansion II

a simple calculation link the function $f_l(k)$ leads to the phase shift

$$f_l(k) = \frac{e^{i2\delta_l} - 1}{2ik} = \frac{1}{k\cot(\delta_l) - ik}. \tag{12}$$

We can take advantage of the partial wave expansion, and write the total scattering cross-section as

$$\sigma = 2\pi \int_{-1}^{1} d(\cos(\theta))|f(\theta,k)|^2 = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l). \tag{13}$$

Using this expression the As a general rule, for a potential decaying as r^{-n} at large distances, for every $l < (n-3)/2$ it holds

$$\delta_l \sim k^{2l+1} \qquad \text{for} \;\; k \to 0. \tag{14}$$

So, for low energy scattering we obtain that the dominant term in the scattering amplitude is $l = 0$. Considering R_{k0}, from trigonometry we have

$$R_{k0} \sim c_1 \frac{\sin(kr)}{kr} + c_2 \frac{\cos(kr)}{r} \qquad \text{for} \;\; r \to \infty, \tag{15}$$

with the condition

$$\tan(\delta_0) = \frac{kc_2}{c_1}. \tag{16}$$

Remember the limit expression $\psi(\mathbf{r}) = 1 - a/r$: neglecting all the contributions except for the s-wave component, we match the expressions and obtain $k \to 0$,

$$a = \lim_{k\to 0}\left(-\frac{\tan(\delta_0)}{k}\right). \tag{17}$$

Keeping only s-wave scattering, we have

$$\sigma = \frac{4\pi}{k^2}\delta_0^2 = 4\pi a^2. \tag{18}$$

T-matrix formalism I

In principle it is possible to derive the δ_l directly from the Schrödinger equation. We show an alternative formalism that allow to obtain useful simplification with respect to this approach. Consider the initial state $|\phi\rangle$, an eigenstate of the free Hamiltonian

$$\hat{H}_0 |\phi\rangle = E |\phi\rangle , \tag{19}$$

and a final state $|\psi\rangle$, eigenstate of the total Hamiltonian, in elastic scattering

$$(\hat{H}_0 + \hat{V}) |\psi\rangle = E |\psi\rangle , \tag{20}$$

so it holds, manipulating the expression

$$(E - \hat{H}_0) |\psi\rangle = \hat{V} |\psi\rangle + (E - \hat{H}_0) |\phi\rangle . \tag{21}$$

Being the operator $\hat{G}_0 = (E - \hat{H}_0)^{-1}$ singular, we specify two class of scattered solutions, $|\psi^{\pm}\rangle$, by defining $\hat{G}_0^{\pm} = (E - \hat{H}_0 \pm i\varepsilon)^{-1}$ for a small, real ε

$$\left|\psi^{\pm}\right\rangle = \hat{V} |\phi\rangle + \hat{G}_0^{\pm} \hat{V} \left|\psi^{\pm}\right\rangle . \tag{22}$$

The scattered states correspond to keeping the outgoing (+) or incoming (-) spherical waves. The above expression is meant to be evaluated keeping the limit $\varepsilon \to 0$, and it is frequently called the **Lippman-Schwinger** equation (in coordinate-free representation). Let the wavevectors of the states $|\phi\rangle$ and $|\phi'\rangle$ be, respectively, $\mathbf{k}$, $\mathbf{k}'$. We can identify the scattering amplitude

$$f(\mathbf{k}', \mathbf{k}) = -\frac{m}{4\pi\hbar^2} \langle\phi'| \hat{V} \left|\psi^+\right\rangle, \tag{23}$$

with θ the angle between the wavevectors of plane wave states $|\phi'\rangle$ (used as a projection) and $|\phi\rangle$. Consider only the outgoing wave solution. We define the **transmission** (T-)**matrix**,

$$\hat{T} |\phi\rangle = \hat{V} \left|\psi^+\right\rangle, \tag{24}$$

whose main advantage is in the writing of

$$f(\mathbf{k}', \mathbf{k}) = -\frac{m}{4\pi\hbar^2} \langle\phi'| \hat{T} |\phi\rangle. \tag{25}$$

Then we can also write

$$f(\mathbf{k}', \mathbf{k}) = -\frac{m}{4\pi\hbar^2} T_{\mathbf{k}'\mathbf{k}}, \tag{26}$$

where $T_{\mathbf{k}'\mathbf{k}} = \langle\phi'|\,\hat{T}\,|\phi\rangle$.
In addition, we have

$$\hat{T}\,|\phi\rangle = \hat{V}\,|\phi\rangle + \hat{V}\hat{G}_0^+\hat{T}\,|\phi\rangle\,, \tag{27}$$

since it holds for every $|\phi\rangle$, this equation holds in an operatorial sense

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0^+\hat{T}. \tag{28}$$

The **Born series** is the expansion of the above equation

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0^+\hat{V} + \hat{V}(\hat{G}_0^+\hat{V})^2 + ... \tag{29}$$

A fundamental approximation can be imposed keeping only the first term. This is the Born approximation

$$\hat{T} \approx \hat{V} \tag{30}$$

In the Born approximation, the scattering length can be expressed readily from the potential, in the limit $k \to 0$

$$a = \frac{m}{4\pi\hbar^2}\int d^3\mathbf{r}\; V(\mathbf{r}). \tag{31}$$

Effective potential I

In the low wavelength limit, scattering is dominated by the s-wave interaction . So we can substitute the potential with an effective one that *reproduces* the correct scattering length. One example, very useful in the calculations, is

$$V_{\text{eff}}(\mathbf{r}) = g_0 \delta^{(3)}(\mathbf{r}). \tag{32}$$

We only need to match

$$V_0 = \int d^3\mathbf{r} V(\mathbf{r}), \tag{33}$$

so to obtain the fundamental relation

$$V_0 = \frac{4\pi\hbar^2}{m} a. \tag{34}$$

But it is possible to make more precise calculations. In fact, the s-wave phase shift can be expanded into

$$k\cot(\delta_0) = -\frac{1}{a} + \frac{1}{2} r k^2, \tag{35}$$

in which the **effective range** r is defined. In an analogous way, we can take an expansion to the second order of the potential in momentum space

$$V(k) = g_0 + g_2 k^2. \tag{36}$$

We characterize the relation between g_0, g_2 and a, r later on. We just notice that this kind of potential corresponds to a real space potential including *delta* functions and derivatives of delta functions.

Effective range correction

$$f(\theta, k) = \frac{1}{k\cot(\delta_0) - ik},$$

$$k\cot(\delta_0) = -\frac{1}{a} + \frac{1}{2}r\ k^2.$$

Now consider how one can include the improved potential into the Gross-Pitaevskii equation. The spatial representation of the potential $V_{\text{eff}}(k) = g_0 + g_2 k^2$ in the relative motion frame is

$$V_{\text{eff}}(\mathbf{r}) = g_0 \delta^{(3)}(\mathbf{r}) + \frac{g_2}{2} \left(\overleftarrow{\nabla}^2 \delta^{(3)}(\mathbf{r}) + \delta^{(3)}(\mathbf{r}) \overrightarrow{\nabla}^2 \right)$$

So we can directly insert this term into the action functional in Hartree approximation, in the presence of a trap potential V_{trap}. We have seen that, for a generic potential,

$$S = N \int dt d^3\mathbf{r} \ \psi(\mathbf{r},t)^* \left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V_{\text{trap}}(\mathbf{r}) - \frac{N-1}{2} \int d^3\mathbf{r}' \ |\psi(\mathbf{r}')|^2 V(\mathbf{r}' - \mathbf{r}) \right] \psi(\mathbf{r},t). \quad (37)$$

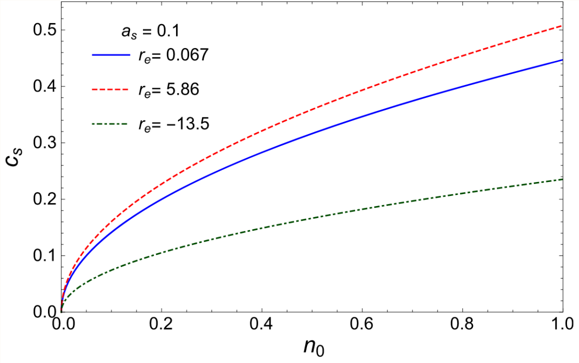
This action is in general nonlocal. By substituting the effective potential, dropping the variables of the wavefunction

$$S = N \int dt d^3\mathbf{r} \ \psi^* \left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - V_{\text{trap}} - \frac{N-1}{2} \left(g_0 |\psi|^2 + \frac{g_2}{2} \nabla^2 |\psi|^2 \right) \right] \psi.$$

Modified Gross-Pitaevskii equation II

We can write the respective Euler-Lagrange equation, called **Modified Gross-Pitaevskii** equation

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}} + g_0(N-1)|\psi|^2 + \frac{g_2}{2}(N-1)\nabla^2|\psi|^2\right]\psi. \quad (38)$$



F. Sgarlata et al. J. Phys. B: At. Mol. Opt. Phys. 48 115301 (2015).

On-shell approximation

The Lippman-Schwinger equation in the momentum space can be written explicitly

$$T_{\mathbf{k}\mathbf{k}'} = V_{\mathbf{k}\mathbf{k}'} + \int d^D\mathbf{k}'' \frac{V_{\mathbf{k}\mathbf{k}''}}{\frac{\hbar^2 k^2}{2m_r} - \frac{\hbar^2 (k'')^2}{2m_r} + i\,\varepsilon} T_{\mathbf{k}''\mathbf{k}'}.$$

We use a generalized partial wave expansion on the equation, and

$$V_{\mathbf{k}\mathbf{k}'} = \frac{1}{(2\pi)^D} \sum_l V_l(k, k')\, N(D, l) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}').$$

We consider only the (generalized) s-wave component

$$T_0(k) = V_0(k) + V_0(k)\; C(k)\; T_0(k),$$

with

$$C(k) = S_D \int_0^\infty \frac{dk''}{(2\pi)^D} \frac{1}{\frac{\hbar^2 k^2}{m} - \frac{\hbar^2 (k'')^2}{m} + i\varepsilon}.$$

The integral for $C(k)$ can be calculated using dimensional regularization

$$C(k) = -\frac{S_D}{(2\pi)^D}\frac{m}{\hbar^2}\int_0^\infty dk''(k'')^{D-1}\frac{1}{(k'')^2+(-ik)^2} = -\frac{m}{\hbar^2}(-ik)^{D-2}\frac{B(D/2,1-D/2)}{(4\pi)^{D/2}\Gamma(D/2)},$$

being B the Euler beta function, that has an integral representation for positive x, y:

$$B(x,y) = \int_0^{+\infty} dt\,\frac{t^{x-1}}{(1+t)^{x+y}},$$

we know that an alternative expression for the beta function is in terms of the gamma function, i.e.

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \tag{39}$$

This allows us to express the beta function even outside the domain ov validity of the integral representation. Using the above equation,

$$C(k) = -\frac{m}{\hbar^2}(-ik)^{D-2}\frac{\Gamma(1-D/2)}{(4\pi)^{D/2}}.$$

Dimensional regularization II

In fact, for $D = 2$, we have the divergent value $\Gamma(0)$. The technique is to use a non-integer dimension $D = 2 - \epsilon$ and let ϵ go to zero only at the end of the calculation. So we start from

$$C(k) = -\frac{m}{\hbar^2}\kappa_0^{\epsilon}(-ik)^{-\epsilon}\frac{\Gamma(\epsilon/2)}{(4\pi)^{1-\epsilon/2}} \; , \quad (40)$$

where the regulator κ_0 is a scale wavenumber. The small-ϵ expansion of the gamma function reads

$$\Gamma(\epsilon/2) = \frac{2}{\epsilon} - \gamma + O(\epsilon) \; , \quad (41)$$

where $\gamma \simeq 0.5572$ is the Euler-Mascheroni constant. Taking into account that

$$x^{\epsilon} = e^{\ln(x^{\epsilon})} = e^{\epsilon \ln(x)} = 1 + \ln(x)\epsilon + O(\epsilon^2),$$

and $\ln(-i) = -i\pi/2$, one gets, after manually removing the remaining singularity

$$C(k) = \frac{m}{2\pi\hbar^2}\ln\left(\frac{k}{2}\frac{e^{\gamma/2}}{\Lambda}\right) - \frac{m}{4\hbar^2}i \; , \quad (42)$$

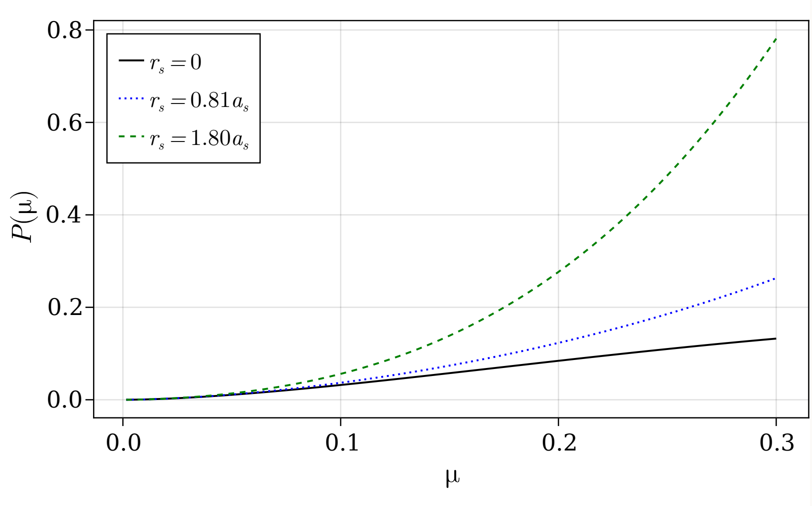
setting $\Lambda = \sqrt{\pi}\kappa_0$, which plays the role of a ultraviolet cutoff.

Results I

Using the regularized $C(k)$, we obtain a systematic link between scattering parameters and the interaction potential expansion, as reported, by connecting our analysis to the values of the scattering amplitudes in all dimensions.

D	$C(k)$	$g_0^* = g_0$	$g_2^* = 2g_2$
3	$-ik\frac{m}{4\pi\hbar^2}$	$\frac{4\pi\hbar^2}{m}a_s$	$\frac{2\pi\hbar^2}{m}a_s^2 r_s$
2	$\frac{m}{2\pi\hbar^2}\ln\left(\frac{k}{2}\frac{e^{\gamma/2}}{\Lambda}\right) - \frac{m}{4\hbar^2}i$	$-\frac{4\pi\hbar^2}{m}\frac{1}{\ln(\Lambda^2 a_s^2 e^{\gamma})}$	$\frac{2\pi^2\hbar^2}{m}\frac{r_s^2}{\ln^2(\Lambda^2 a_s^2 e^{\gamma})}$
1	$-i\frac{1}{k}\frac{m}{2\hbar^2}$	$-\frac{2\hbar^2}{m a_s}$	$-\frac{\hbar^2}{m}r_s$

Results II



preprint: F. Lorenzi, A. Bardin, L. Salasinch, arXiv 2303.02675 (2023).

Multi-channel scattering

Multi-channel scattering I

Consider two alkali atoms, with nuclear spins I_1 and I_2. Since $S = 1/2$, we have a total of $4(2I_1 + 1)(2I_2 + 1)$ hyperfine states. The scattering event can couple those states together. In a general setting, the Hamiltonian of the system, in the relative motion frame, is

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{43}$$

where

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m_r} + \hat{H}_{\mathsf{spin},1} + \hat{H}_{\mathsf{spin},2}, \tag{44}$$

let greek letter states denote eigenstates of spin Hamiltonians

$$\hat{H}_{\mathsf{spin}} \left|\alpha\right\rangle = \epsilon_\alpha \left|\alpha\right\rangle .$$

Energy eigenstates are denoted by

$$E_{\alpha\beta}(k_{\alpha\beta}) = \frac{\hbar^2 k_{\alpha\beta}^2}{2m_r} + \epsilon_\alpha + \epsilon_\beta.$$

Multi-channel scattering II

We use the asymptotic expansion of the wavefunction

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_{\alpha\beta}\cdot\mathbf{r}} |\alpha\beta\rangle + \sum_{\alpha'\beta'} f_{\alpha\beta}^{\alpha'\beta'}(\mathbf{k}_{\alpha\beta}, \mathbf{k}'_{\alpha'\beta'}) \frac{e^{-k'_{\alpha'\beta'}r}}{r} |\alpha'\beta'\rangle \,, \tag{45}$$

the incoming spin state is called the **entrance channel**, and the outgoing one **exit channel**. Since the channels have different spin energies, the wavenumbers must satisfy

$$\frac{\hbar^2 k'^2_{\alpha'\beta'}}{2m_\mathrm{r}} = \frac{\hbar^2 k^2_{\alpha\beta}}{2m_\mathrm{r}} + \epsilon_\alpha + \epsilon_\beta - \epsilon_{\alpha'} - \epsilon_{\beta'},$$

if this imply that $k'^2_{\alpha'\beta'} \leq 0$ the channel is called **closed channel**. We define also the **threshold energy**

$$E_\mathrm{th}(\alpha'\beta') = \epsilon_{\alpha'} + \epsilon_{\beta'}. \tag{46}$$

Feshbach resonance I

Consider the space of all states to be divided into P, the subspace of open channels, and Q the subspace of closed channels. Then a generic wavefunction is

$$|\psi\rangle = |\psi_P\rangle + |\psi_Q\rangle \,.$$

Consider $\mathcal{P}$ and $\mathcal{Q}$ the projectors onto the respective subspaces. Let us multiply the Schrödinger equation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle \,,$$

by projectors

$$(E - \hat{H}_{PP})\,|\psi_P\rangle = \hat{H}_{PQ}\,|\psi_Q\rangle$$
$$(E - \hat{H}_{QQ})\,|\psi_Q\rangle = \hat{H}_{QP}\,|\psi_P\rangle \,,$$

using the usual prescription for $i\varepsilon$, solving formally the second equation

$$|\psi_Q\rangle = (E - \hat{H}_{QQ} + i\varepsilon)^{-1}\hat{H}_{QP}\,|\psi_P\rangle \,,$$

Feshbach resonance II

and substituting into the first one

$$(E - \hat{H}_{PP} - \hat{H}'_{PP})\,|\psi_P\rangle = 0,$$

where

$$\hat{H}'_{PP} = \hat{H}_{PQ}(E - \hat{H}_{QQ} + i\varepsilon)^{-1}\hat{H}_{QP}.$$

Let

$$\hat{H}_{PP} = \hat{H}_0 + \hat{V}_1,$$

where $\hat{V}_1$ is the potential in the open channel. We can rewrite the equation for $|\psi_P\rangle$ in a more physical way

$$(E - \hat{H}_0 - \hat{V})\,|\psi_P\rangle = 0,$$

where we have defined the **effective interaction** operator in the subspace of open channels as

$$\hat{V} = \hat{V}_1 + \hat{V}_2,$$

and the additional interaction due to the coupling to the closed channel

$$\hat{V}_2 = \hat{H}'_{PP},$$

Consider the T-matrix equaition $\hat{T} = \hat{V} + \hat{V}\hat{G}_0^+\hat{T}$, with formal solution

$$\hat{T} = \hat{V}(1 - \hat{V}\hat{G}_0^+)^{-1} = (1 - \hat{G}_0^+\hat{V})^{-1}\hat{V}. \tag{47}$$

We can simplify to

$$\hat{T} = (E - \hat{H}_0 + i\varepsilon)(E - \hat{H}_0 - \hat{V} + i\varepsilon)^{-1}\hat{V}. \tag{48}$$

Define $\hat{B} = \hat{V}_2$, $\hat{A} = E - \hat{H}_0 - \hat{V}_1 + i\varepsilon$. Then

$$\hat{T} = (E - \hat{H}_0 + i\varepsilon)(\hat{A} - \hat{B})^{-1}\hat{V}, \tag{49}$$

now consider the operator identity

$$(\hat{A} - \hat{B})^{-1} = \hat{A}^{-1}(1 + \hat{B}(\hat{A} - \hat{B})^{-1}). \tag{50}$$

We get a modified equation for the total T-matrix

$$\hat{T} = \hat{T}_1 + (1 - \hat{V}_1 \hat{G}_0^+)^{-1} \hat{V}_2 (1 - \hat{G}_0^+ \hat{V})^{-1} \tag{51}$$

$$\hat{T}_1 = \hat{V}_1 + \hat{V}_1 \hat{G}_0^+ \hat{T}. \tag{52}$$

Let us take matrix elements using the plane wave states $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$. Suppressing channel indexes in the T-matrix elements, we write

$$T_{\mathbf{k}'\mathbf{k}} = T_{1,\mathbf{k}'\mathbf{k}} + \langle \mathbf{k}'| (1 - \hat{V}_1 \hat{G}_0^+)^{-1} \hat{V}_2 (1 - \hat{G}_0^+ \hat{V})^{-1} |\mathbf{k}\rangle , \tag{53}$$

one can notice that the state $(1 - \hat{G}_0^+ \hat{V})^{-1} |\mathbf{k}\rangle$ is an eigenstate of $\hat{H}_0 + \hat{V}$. We may denonte this state with $\left|\mathbf{k}; \hat{V}, +\right\rangle$ In a similar way, using

$$\langle \mathbf{k}'| (1 - \hat{V}_1 \hat{G}_0^+)^{-1} = [(1 - \hat{G}_0^- \hat{V}_1)^{-1} |\mathbf{k}'\rangle]^\dagger,$$

we have the right state represented by an incoming wave. These states are no more plane waves, but they are transformed by the interactions. We can also approximate $\hat{V}$ inside the second term with $\hat{V}_1$, thus calculating the first order correction in $\hat{V}_2$. Finally, let us go to the limit $k \to 0$. We can define a_P as the scattering length in the P space, and using $|\psi_n\rangle$ eigenstates of $\hat{H}_{QQ}$, we obtain, from the full expression of $\hat{V}_2$,

$$\hat{V}_2 = \hat{H}'_{PP} = \hat{H}_{PQ}(E - \hat{H}_{QQ} + i\varepsilon)^{-1}\hat{H}_{QP},$$

the relation

$$\frac{4\pi\hbar^2}{m}a = \frac{4\pi\hbar^2}{m}a_P + \sum_n \frac{|\langle\psi_n|\,\hat{H}_{QP}\,|\psi_0\rangle|^2}{E_{th} - E_n}, \tag{54}$$

the nonresonant terms into the are almost constant with energy, so we incorporate all terms into consider only the resonant state

$$\frac{4\pi\hbar^2}{m}a = \frac{4\pi\hbar^2}{m}a_{bg} + \frac{|\langle\psi_{\text{res}}|\,\hat{H}_{QP}\,|\psi_0\rangle|^2}{E_{th} - E_{\text{res}}}, \tag{55}$$

$$E_{th} - E_{\text{res}} \approx (\mu_{\text{res}} - \mu_\alpha - \mu_\beta)(B - B_0), \tag{56}$$

Feshbach resonance VI

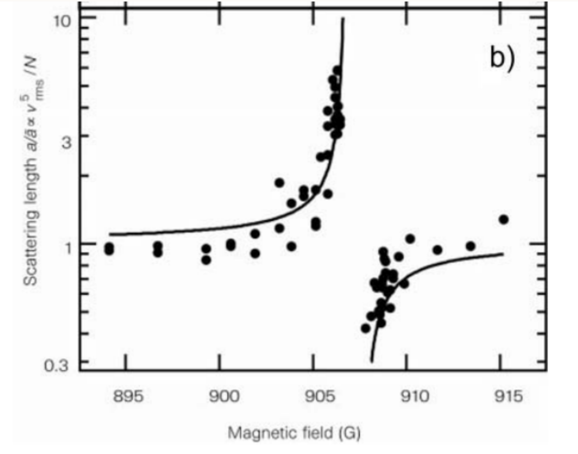
and we recollect the usual formula for Feshbach resonance

$$a(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right). \tag{57}$$

with

$$\Delta B = \frac{m}{4\pi\hbar^2 a_{bg}} \frac{|\langle\psi_{\mathsf{res}}|\,\hat{H}_{QP}\,|\psi_0\rangle|^2}{\mu_{\mathsf{res}} - \mu_\alpha - \mu_\beta}.$$

Feshbach resonance VII



S. Inouye et. al, Nature 392, 151–154 (1998).

Additional material

Boltzmann transport equation

Suppose we are at $T > T_C$, and $kT >> \Delta E$, the level spacing of the trap potential. Suppose also to neglect the mean-field potential since $kT >> nU_0$. Then we can use a semiclassical distribution of states f, obeying the Bolzmann equation.

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t} \right)_{\text{source}} \tag{58}$$

The source term is given by the interactions, in particular it depends on the scattering cross section $\sigma = 8\pi a^2$, and uses the principle of detailed balance (assuming only s-wave interaction). By linearizing the equation, we get damping of the oscillation modes imposed by the interaction.

Hyperfine and Zeeman Hamiltonian

$$\hat{H}_{\mathsf{spin}} = A\mathbf{I}\cdot\mathbf{J} + CJ_z + DI_z$$