Universality and effective range corrections in quantum gases: from scattering parameters to the effective potential

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[F. Lorenzi, A. Bardin, and L. Salasnich, Phys. Rev. A 107, 033325 (2023)]

CMD30/FisMat2023,
Quantum gases as analogues of condensed matter systems
Milano, September 5 2023

Dipartimento di Fisica e Astronomia
"Galileo Galilei"

Università degli Studi di Padova

Outline of the talk

1. Introduction and motivation

2. Framework of scattering theory

3. Effective range correction

4. Some applications

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Interactions in a quantum gases

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- In cold atomic gases the interparticle spacing is typically an order of magnitude larger than length scale of the interaction $\longrightarrow$ for a large class of systems only two-body interactions are relevant.
- 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 internal states due to scattering may induce trap loss. We considere here only single-channel scattering.
- It is not in general possible to make very precise theoretical calculation for the shape of the potentials $\longrightarrow$ in Monte Carlo simulations we use some model potentials that are related to specific scattering parameters.

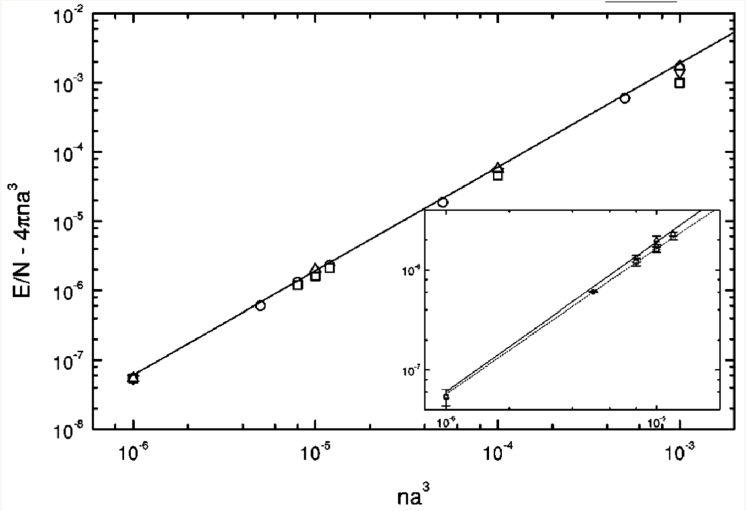
For example

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

Universality in quantum gases

Regardless of the actual shape of the potential, the interactions can be completely described by a single parameter: the s-wave scattering length a_s.

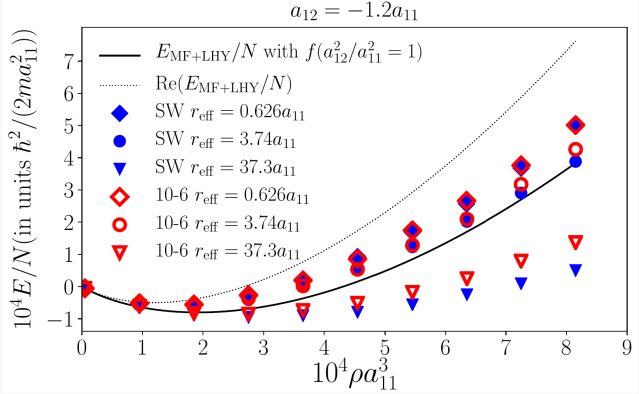
Universality in quantum gases 2



S. Giorgini et al., Phys. Rev. A 60, 6 (1999)

Evidences of nonuniversality

In some recent DMC calculations, it has been shown for Bose-Bose mixtures that the universal description is not always successful in describing the gas properties.



V. Cikojevic et al., Phys. Rev. A 99, 2 (2019).

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T-matrix formalism

We define the transmission (T-)matrix,

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

by using plane waves, eigenstates of the momentum operator, we can express the scattering length from the T-matrix

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

where $T_{\mathbf{k}'\mathbf{k}} = \left\langle\phi'\right|\hat{T}\left|\phi\right\rangle$.

In addition, we have the Lippman-Schwinger equation

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

T-matrix formalism 2

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

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

The Born series is the expansion of the above equation

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

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

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

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

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

Effective potential

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

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

Expressing the coefficient as

$$g_0 = \int d^3\mathbf{r} V_{\text{eff}}(\mathbf{r}),$$

we can easily match the result to the effective range a_s

$$g_0 = \frac{4\pi\hbar^2}{m} a_s.$$

Effective potential 2

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

$$k \cot(\delta_0) = -\frac{1}{a_s} + \frac{1}{2} r_s k^2,$$

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

$$V_{\text{eff}}(k) = g_0 + g_2 k^2.$$

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

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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 s-wave projection, and, considering the diverging behaviour of of the integral argument for small ε, asssume an on-shell approximation:

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

with

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

Dimensional regularization

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.

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

Dimensional regularization 2

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

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

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

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

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

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

Dimensional regularization 3

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 removing the singularity

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

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

Results

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	$-i\frac{1}{k}\frac{m}{2\hbar^2}$	$-\frac{2\hbar^2}{m a_s}$	$-\frac{\hbar^2}{m}r_s$

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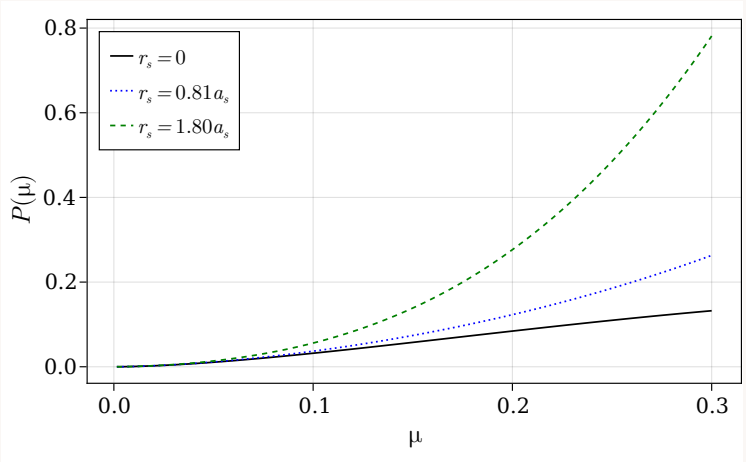
Zero temperature two-dimensional Bose gas pressure

$$P(\mu) = \frac{m}{8\pi\hbar^2}\mu^2 \ln\left(\frac{4\hbar^2}{m\mu a_s^2 e^{2\gamma+1/2}}\right) + \frac{3m^2}{16\hbar^4} r_s^2\ \mu^3$$



Modified Gross-Pitaevskii equation

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,

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

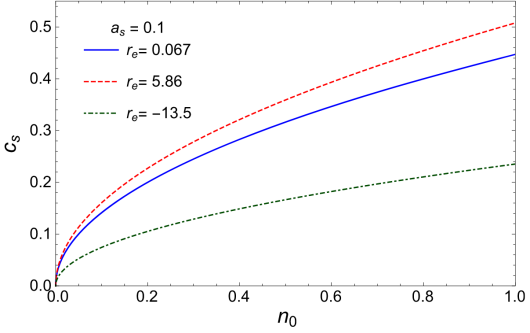
This action is in general nonlocal. By substituting the effective potential, dropping the variables of the wavefunction

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

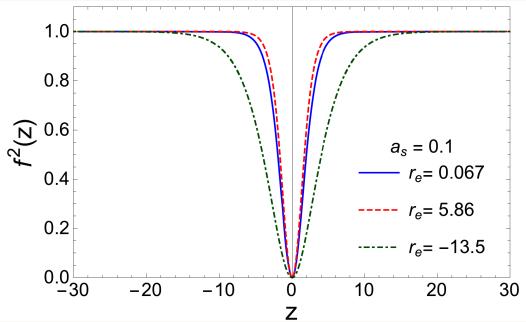
Modified Gross-Pitaevskii equation 2

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

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



Modified Gross-Pitaevskii equation 3



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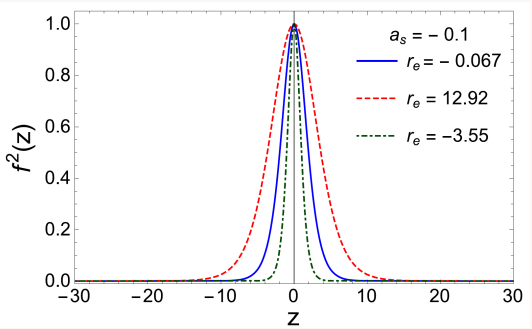

(b)

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Conclusions and open problems

- Universal description of the Bose gas is an extremely powerful tool, but it can fail in particular physical systems.
- Non-universal corrections in the low-energy limit can be calculated, as we have shown, by using both s-wave and on-shell approximations .

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Further results to achieve

- Generalize the treatment to fully address atomic mixtures.
- Compute effective range corrections in the context of atomic Josephson junctions in reduced spatial dimensions.

Thank you for the attention!

F. Lorenzi, A. Bardin, and L. Salasnich, Phys. Rev. A 107, 033325 (2023)

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Additional material

The discrepancy in the literature for the 3D case

By computing the s-wave phase shift from the energy shift (Collin, Massignan and Pethick), one obtains

$$g_2 \propto \frac{a_s^3}{3} - \frac{a_s r_s}{2}.$$

Instead, by using an effective field theory and matching the low-energy observables (Braaten and Hammer), one obtains

$$g_2 \propto a_s^2 r_s$$

As a puzzling consequence, we have that in the energy shift approach, even sending the effective range to zero, the g_2 correction stays finite.

E. Braaten, H.-W. Hammer, and S. Hermans, Phys. Rev. A 63, 6 (2001).
A. Collin, P. Massignan, and C. J. Pethick, Phys. Rev. A 75, 1 (2007).

Scattering amplitude and partial wave expansion

Two-body problem

Let us consider the motion of two distinguishable particles of the same mass m in a unit volume, in presence of an interaction potential depending only on the distance between the particles. We consider 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

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

and 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.

s-wave scattering length from scattering amplitude

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 $f(\theta) =: -a$,

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

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

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

s-wave scattering length from scattering amplitude 2

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

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

For identical particles, one must impose symmetry and antisymmetry for the bosonic and fermionic case, and the scattering cross section becomes doubled for Bosons, and zero for Fermions. Fermions are not subjected to the s-wave scattering.

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

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

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

$$z \to -z, \tag{1}$$

$$\theta \to \pi - \theta, \tag{2}$$

so symmetrized/antisymmetrized wavefunction is

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

Scattering of identical particles 2

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

$$\sigma = 8\pi a^2,$$

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

Partial wave expansion

The wavefunction can be expanded in *partial waves*

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

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

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

the asymptotic solution reads

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

Partial wave expansion 2

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

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

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

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

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

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

Partial wave expansion 3

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

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

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

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

with the condition

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

Remember the limit expression $\psi(\mathbf{r}) = 1 - a/r$: neglecting all the contributions except for

Partial wave expansion 4

the s-wave component, we match the expressions and obtain $k \to 0$,

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

Keeping only s-wave scattering, we have

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

T-matrix formalism

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

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

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

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

so it holds, manipulating the expression

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

T-matrix formalism 2

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

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

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

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

with θ the angle between the wavevectors of plane wave states $|\phi'\rangle$ (used as a projection) and $|\phi\rangle$.

s-wave T-matrix and phase shift in all dimensions

In 3D case:

$$T_0(k) = -\left(\frac{4\pi\hbar^2}{m}\right)\left(\frac{1}{k\cot(\delta_0(k)) - ik}\right) .$$

In 2D case:

$$T_0(k) = -\left(\frac{4\hbar^2}{m}\right)\left(\frac{1}{\cot(\delta_0(k)) - i}\right) .$$

In 1D case:

$$T_0(k) = -\left(\frac{2\hbar^2}{m}\right)\left(\frac{k}{\cot(\delta_0(k)) - i}\right) .$$

Multi-channel scattering

Multi-channel scattering

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

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

where

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

let greek letter states denote eigenstates of spin Hamiltonians

$$\hat{H}_{\text{spin}} |\alpha\rangle = \epsilon_\alpha |\alpha\rangle .$$

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 2

We use the asymptotic expansion of the wavefunction

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

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

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

Feshbach resonance

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

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

Feshbach resonance 2

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

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

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

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

Feshbach resonance 3

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

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

Feshbach resonance 4

We can simplify to

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

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

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

now consider the operator identity

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

We get a modified equation* for the total T-matrix

$$\hat{T} = \hat{T}_1 + (1 - \hat{V}_1\hat{G}_0^+)^{-1}\hat{V}_2(1 - \hat{G}_0^+\hat{V})^{-1} \tag{3}$$

$$\hat{T}_1 = \hat{V}_1 + \hat{V}_1\hat{G}_0^+\hat{T}. \tag{4}$$

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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

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

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

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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

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

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

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

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

and we recollect the usual formula for Feshbach resonance

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

with

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

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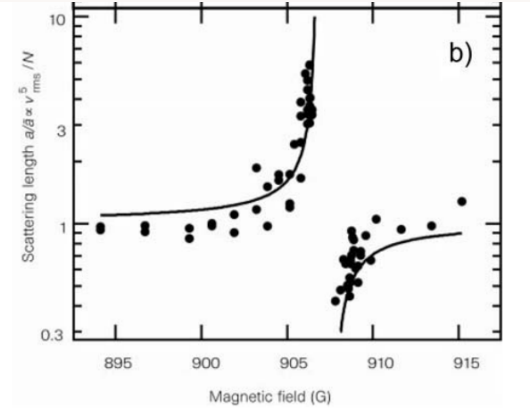

S. Inouye et. al, Nature 392, 151–154 (1998).

Other 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*.

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

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

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