An introduction to low-energy scattering in quantum mechanics

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References

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Scattering length and effective range of microscopic two-body potentials

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- Or your favorite quantum mechanics textbook: Griffiths, Sakurai, ...

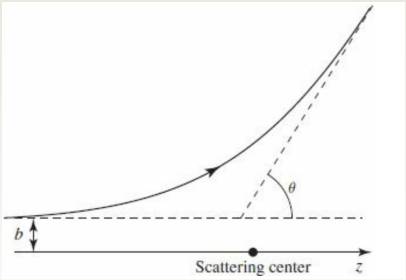
Motivation

- Scattering processes are a fundamental way of experimentally probing distributions and properties of systems in several areas of physics
  - Can you name a few examples?
- Low-energy quantum scattering theory
  - What is low-energy?

Introduction

- What is scattering?
  - Scattering is the interaction of an object with a scattering center
    - classical particle
    - electromagnetic wave
    - **quantum particle**
  - scattering potential

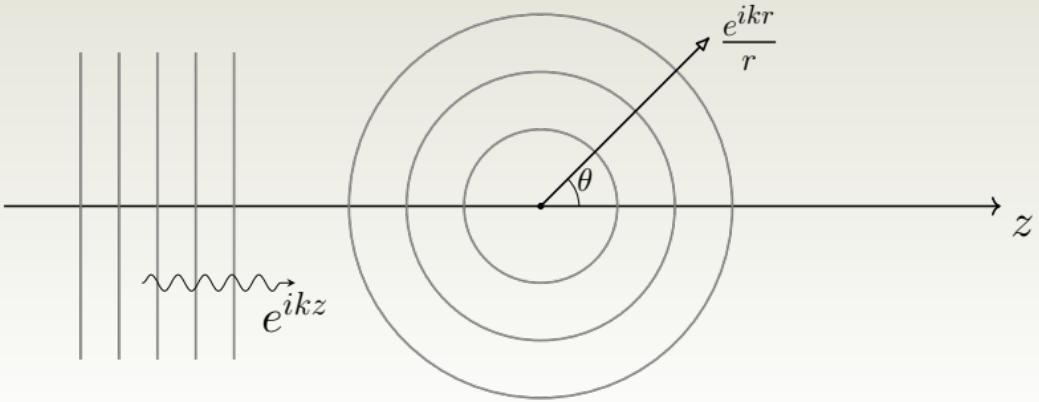
- Classical view



Griffiths

Introduction

- Quantum view



Quantum scattering theory

- Hypotheses
  1. Elastic scattering
  2. Incident plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$
  3. Local and finite-ranged potential

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow{\text{large } r} \mathcal{N}\left[e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f(\mathbf{k}', \mathbf{k})\right]$$

Quantum scattering theory

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- Formally, in quantum mechanics, a scattering process is described as a transition from one quantum state to another

$$|i\rangle \to |f\rangle$$

- Assume $|i\rangle$ to be a plane wave $|\mathbf{k}\rangle$, that is, a free particle

$$H_0|i\rangle = E_i|i\rangle = \frac{\hbar^2\mathbf{k}^2}{2m}|\mathbf{k}\rangle$$

- Scattering is taken into account by introducing a potential $V(\mathbf{r})$

$$H = H_0 + V(\mathbf{r})$$

Quantum scattering theory

- Quantization of the scattering states

$$\langle \mathbf{r}|\mathbf{k}\rangle = \mathcal{N} e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}}$$

- We must take $L \to \infty$ to guarantee the continuum character of the state at the end of our calculations

Quantum scattering theory

- More hypotheses
  1. Elastic scattering
  2. Incident plane wave in the z direction: e^{ikz}
  3. Local, finite-ranged and spherically-symmetric potential $V(r)$

$$\psi_{\mathbf{k}}(r,\theta) \xrightarrow{\text{large } r} \mathcal{N}\left[e^{ikz} + \frac{e^{ikr}}{r} f(\theta)\right]$$

- The finite range of the potential (and spherical symmetry) invite us to solve the Schrödinger equation for $V(0 < r < R) \neq 0$ and $V(r > R) = 0$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi$$

Spherical coordinates

- Due to the spherical symmetry of $V(r)$, it is convenient to employ spherical coordinates

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{L^2}{2mr^2}+V(r)\right)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

- L is the angular momentum operator

$$L^2=-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

- Its z-component is given by

$$L_z=-i\hbar\frac{\partial}{\partial\phi}$$

- Construct a complete set of eigenfunctions related to H, L^2, and L_z

$$\begin{aligned}H\psi(r,\theta,\phi)&=E\psi(r,\theta,\phi),\\ L^2\psi(r,\theta,\phi)&=l(l+1)\hbar^2\psi(r,\theta,\phi),\\ L_z\psi(r,\theta,\phi)&=m\hbar\psi(r,\theta,\phi)\end{aligned}$$

Spherical coordinates

- We propose a separable solution of the form

$$\psi(r,\theta,\phi) = A_l(r)Y_l^m(\theta,\phi)$$

- To avoid taking the first radial derivative of $A_l(r)$, we define the "reduced" radial solution $u_l(r) = rA_l(r)$

$$\left(\frac{d^2}{dr^2} + k^2 - U(r) - \frac{l(l+1)}{r^2}\right) u_l(r) = 0$$

  - $k^2 = 2mE/\hbar^2$
  - $U(r) = 2mV(r)/\hbar^2$
  - $l(l+1)$ is the "separation constant"

Solution for $r > R$

- Outside the potential range R, we must solve

$$\left(\frac{d^2}{dr^2} + k^2 - \cancel{U(r)}^{\,0} - \frac{l(l+1)}{r^2}\right) u_l(r) = 0$$

- The solution for $r > R$ can be written in terms of the spherical Bessel functions $j_l(x)$ and $n_l(x)$

$$u_l(r) = c_l' r j_l(kr) + c_l'' r n_l(kr)$$

- $j_0(x) = \frac{\sin(x)}{x}$
- $j_1(x) = \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}$
- $j_2(x) = \frac{3\sin(x)}{x^3} - \frac{3\cos(x)}{x^2} - \frac{\sin(x)}{x}$

- $n_0(x) = -\frac{\cos(x)}{x}$
- $n_1(x) = -\frac{\cos(x)}{x^2} - \frac{\sin(x)}{x}$
- $n_2(x) = -\frac{3\cos(x)}{x^3} - \frac{3\sin(x)}{x^2} + \frac{\cos(x)}{x}$

Spherical Bessel functions

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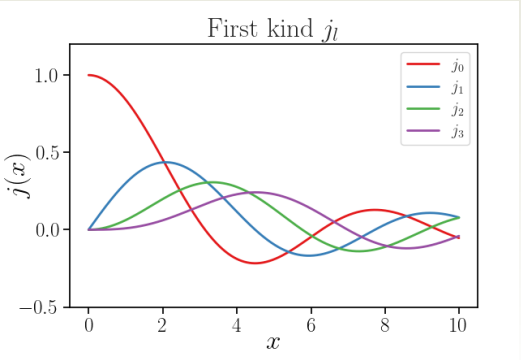
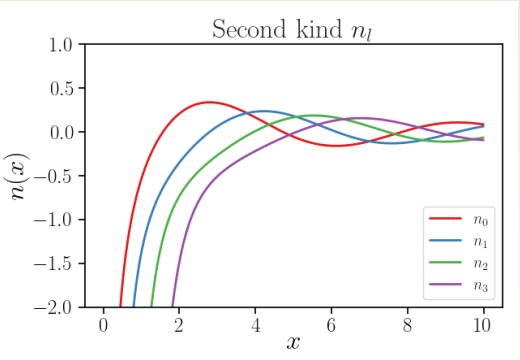




Spherical Hankel functions

- $j_l(x)$ and $n_l(x)$ are generalized sines and cosines
- It is more convenient to write the solution in terms of e^{ikx}/x to represent "incoming" or "outgoing" spherical waves
- Similarly to $e^{ix} = \cos(x) + i\sin(x)$, we define the spherical Hankel functions as

$$h_l^{(1)}(x) = j_l(x) + i n_l(x)$$
$$h_l^{(2)}(x) = j_l(x) - i n_l(x)$$

- $h_0^{(1)}(x) = -\frac{ie^{ix}}{x}$
- $h_1^{(1)}(x) = -e^{ix}\,\frac{x+i}{x^2}$
- $h_2^{(1)}(x) = i\,e^{ix}\,\frac{x^2+3ix-3}{x^3}$
- $h_0^{(2)}(x) = \frac{ie^{-ix}}{x}$
- $h_1^{(2)}(x) = -e^{-ix}\,\frac{x-i}{x^2}$
- $h_2^{(2)}(x) = -i\,e^{-ix}\,\frac{x^2-3ix-3}{x^3}$

- The solution for $u_l(r)$ can be written as

$$u_l(r) = c_l^{(1)} r h_l^{(1)}(kr) + c_l^{(2)} r h_l^{(2)}(kr)$$

Free particle solution

- The free particle solution in cartesian coordinates is a plane wave e^{ikz}
- In spherical coordinates, $e^{ikz} = e^{ikr\cos\theta}$ contains all possible values of l. This can be expressed with Rayleigh's formula:

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

- Note that only j_l appears. Physically, this is due to the divergence of $n_l(kr)$ at $r = 0$.
- In terms of the spherical Hankel functions,

$$j_l(x) = \frac{h_l^{(1)}(x) + h_l^{(2)}(x)}{2}$$

Asymptotic behavior

- Let us analyze the asymptotic behavior, that is, when $r \to \infty$

$$h_l^{(1)}(x) \xrightarrow{\text{large } x} (-i)^{l+1} \frac{e^{ix}}{x},$$
$$h_l^{(2)}(x) \xrightarrow{\text{large } x} i^{l+1} \frac{e^{-ix}}{x}.$$

- The free-particle solution at $r \to \infty$ is

$$e^{ikr\cos\theta} \xrightarrow{\text{large } r} \sum_{l=0}^{\infty} \frac{(2l+1)}{2ikr} \left[e^{ikr} - (-1)^l e^{-ikr}\right] P_l(\cos\theta).$$

- The first term inside the square brackets represents an outgoing spherical wave, while the second is related to an incoming spherical wave.

Asymptotic behavior

- Motivated by the expansion for $e^{ikr\cos\theta}$, we write the scattered solution for every $r > R$ as

$$\psi(r,\theta) = \mathcal{N}\sum_{l=0}^{\infty} i^l(2l+1)\frac{u_l(r)}{r}P_l(\cos\theta)$$

- And the asymptotic behavior

$$\psi(r,\theta) \xrightarrow{\text{large } r} \mathcal{N}\sum_{l=0}^{\infty}\frac{(2l+1)}{ikr}\left[c_l^{(1)}e^{ikr} - (-1)^l c_l^{(2)}e^{-ikr}\right]P_l(\cos\theta) \qquad (*)$$

- Let us compare with

$$e^{ikr\cos\theta} \xrightarrow{\text{large } r} \sum_{l=0}^{\infty}\frac{(2l+1)}{2ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right]P_l(\cos\theta) \qquad (**)$$

- $(**)$ describes the asymptotic behavior of the wave function for a plane wave without being scattered, while $(*)$ does the same, but in a situation where scattering could have taken place.

Phase shift

- We introduce a new quantity related to the ratio between the constants

$$\frac{c_l^{(1)}}{c_l^{(2)}} = S_l(k) = e^{2i\delta_l(k)}$$

- Expressing the asymptotic wave function in terms of the phase shift

$$\psi(r,\theta) \xrightarrow{\text{large } r} \mathcal{N} \sum_{l=0}^{\infty} \frac{(2l+1)}{ikr} c_l^{(2)} \left[e^{2i\delta_l} e^{ikr} - (-1)^l e^{-ikr} \right] P_l(\cos\theta)$$

- Now we have everything we need to connect with the asymptotic wave function obtained before we restricted to spherically-symmetric potentials

Phase shift

- We know that

$$\psi_{\mathbf{k}}(r,\theta) \xrightarrow{\text{large } r} \mathcal{N}\left[e^{ikz} + \frac{e^{ikr}}{r} f(\theta)\right]$$

- Expanding e^{ikz}

$$\psi_{\mathbf{k}}(r,\theta) \xrightarrow{\text{large } r} \mathcal{N}\left\{\left[\sum_{l=0}^{\infty} \frac{(2l+1)}{2ikr}\left(e^{ikr} - (-1)^l e^{-ikr}\right) \times P_l(\cos\theta)\right] + f(\theta)\frac{e^{ikr}}{r}\right\}$$

- Comparing with

$$\psi(r,\theta) \xrightarrow{\text{large } r} \mathcal{N}\sum_{l=0}^{\infty} \frac{(2l+1)}{ikr} c_l^{(2)}\left[e^{2i\delta_l} e^{ikr} - (-1)^l e^{-ikr}\right] P_l(\cos\theta)$$

Phase shift

- Collecting the terms with e^{ikr} allows us to write the scattering amplitude as a function of the phase shift

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

- The factor $(e^{2i\delta_l} - 1)/2ik$ is referred to as the partial wave amplitude $f_l(k)$, which may be rewritten as

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

- In terms of $S_l(k)$

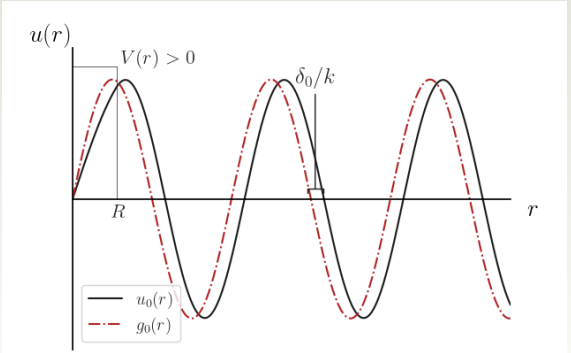
$$S_l(k) = 1 + 2ikf_l(k) = e^{2i\delta_l(k)}$$

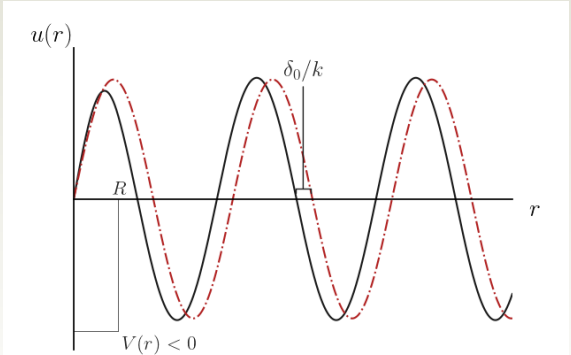
Physical meaning of the phase shift

- $\delta_l(k)$ is the difference between the phases of the incident and the scattered function
- The probability is conserved during the scattering
  - The only thing that can change is the phase of the wave function
- If $V = 0$: free particle
  - $\delta_l(k) = 0, f_l(k) = 0$
- If $V \neq 0$: solution for $r < R$ depends on the details of V
  - but for $r > R$ we have a free particle with a "shifted" phase
- Defining the phase shift allows us to reduce the scattering problem to calculate a single quantity, $\delta_l(k)$

Physical meaning of the phase shift

- $g_0(r)$ is the free-particle solution
- $u_0(r)$ is the solution in the presence of a scattering potential





- A repulsive potential ($V > 0$) "pushes" the particle away
- An attractive potential ($V < 0$) "pulls" the particle towards the origin

Computing the phase shift

- Logarithmic derivative

$$\frac{d}{dx}\ln f(x) = \frac{f'(x)}{f(x)}.$$

- To compute the phase shift, we define the dimensionless ratio $r \times u'(r)/u(r)$

$$\beta_l = \left[r\frac{u_l'(r)}{u_l(r)} \right]_{r=R^-}$$

  - $R^{\pm} \equiv \lim_{\epsilon\to 0} R \pm \epsilon$

- The radial solution at $r > R$ is

$$u_l(r) = \frac{1}{2} r e^{2i\delta_l} h_l^{(1)}(kr) + \frac{1}{2} r h_l^{(2)}(kr) = r e^{i\delta_l}(\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr))$$

Computing the phase shift

- Equating β_l with the outside log solution (at $r = R^+$):

$$\beta_l = \left[r \frac{u_l'(r)}{u_l(r)} \right]_{r=R^+} = 1 + kR \left[\frac{\cos\delta_l j_l'(kR) - \sin\delta_l n_l'(kR)}{\cos\delta_l j_l(kR) - \sin\delta_l n_l(kR)} \right],$$

- After some algebra, we arrive at an expression for the phase shift

$$\cot\delta_l(k) = \frac{kR\, n_l'(kR) - (\beta_l - 1)\, n_l(kR)}{kR\, j_l'(kR) - (\beta_l - 1)\, j_l(kR)}$$

Low-energy limit

- From the radial equation for any partial wave l

$$\left(\frac{d^2}{dr^2} + k^2 - U(r) - \frac{l(l+1)}{r^2}\right) u_l(r) = 0$$

- We define an effective potential for the l-th partial wave as

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

- For $l \neq 0$, we a have repulsive centrifugal barrier
- If the reduced wavelength $\lambda\!\!\!^{-} = \lambda/2\pi = 1/k$ of the incident wave is much larger than the potential range, that is $\lambda\!\!\!^{-} \gg R$ or $kR \ll 1$, then the particle cannot overcome the centrifugal barrier
- In this case, the partial waves with $l > 0$ are unimportant, and the $l = 0$ component is dominant in understanding low-energy scattering

s-wave scattering

- In the low-energy scenario, we consider partial waves with $l \neq 0$ to vanish, and the resulting $l = 0$ term is referred to as "s-wave"
- The s-wave radial component, which we denote by $u_0^{(k\neq 0)}(r)$, is given by

$$\begin{aligned} A_0^{(k\neq 0)}(r) = \frac{u_0^{(k\neq 0)}}{r} &= e^{i\delta_0}(\cos\delta_0 j_0(kr) - \sin\delta_0 n_0(kr)) \\ &= e^{i\delta_0}\left[\frac{1}{kr}\sin(kr+\delta_0)\right] \end{aligned}$$

s-wave scattering

- We can also solve the zero-energy Schrödinger's equation, that is $k = 0$, at $r > R$:

$$\left(\frac{d^2}{dr^2} + \cancel{k^2}^{0} - \cancel{U(r)}^{0} - \cancel{\frac{l(l+1)}{r^2}}^{0} \right) u_0^{(k=0)}(r) = 0$$

- We simply have $u_0''^{(k=0)}(r) = 0$
- The solution can be written as $u_0^{(k=0)}(r) = c(r - a)$
- Its logarithmic derivative is

$$r \frac{u_0'^{(k=0)}(r)}{u_0^{(k=0)}(r)} = \frac{r}{r-a}.$$

- This needs to be equal to the log derivative of $u_0^{(k\neq 0)}(r)$

$$kr \cot(kr + \delta_0) = \frac{r}{r-a}$$

Scattering length

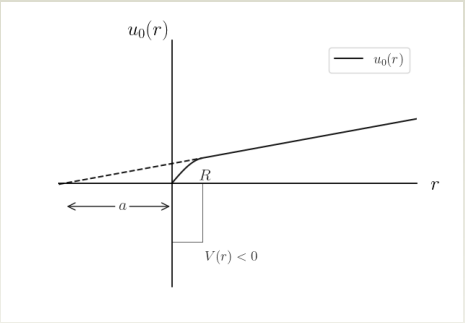
- In the limit $k \to 0$, and also setting $r = 0$, we define the scattering length a

$$\lim_{k \to 0} k \cot \delta_0(k) = -\frac{1}{a}$$

- We reduced the scattering problem to calculating $\delta_l(k)$. Now we reduced the problem even further: in the $E \approx 0$ limit, a encodes all the information we need about scattering.
- Geometrical interpretation: choose $c = -1/a$ in

$$u_0^{(k=0)}(r) = 1 - \frac{r}{a}$$

- a is simply the intercept of the outside wave function with the x-axis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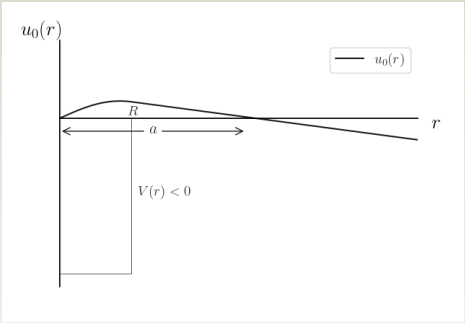
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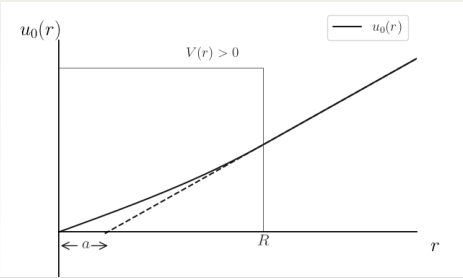

$u_0(r)$
$u_0(r)$
$V(r) > 0$
a
R
r

The effective range

- Another name for the scattering length expansion is the zero-range expansion
- What happens if the range of the potential is small, but non-negligible?
- We need the next term of the expansion in powers of k of $k \cot \delta_0(k) = -1/a$
- $k \cot \delta_0(k)$ is an even function, thus the next term is certainly not linear in k
- The result is

$$k \cot \delta_0(k) = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \mathcal{O}(k^4)$$

The effective range

- Consider a different normalization for $u_0(r > R)$

$$u_0(r > R) = \cot\delta_0(k)\sin(kr) + \cos(kr)$$

- Let us take the $l = 0$ radial equation, for two different wave functions $u_{k_1}(r)$ and $u_{k_2}(r)$, labeled by their wave vectors $k_1 = \sqrt{2mE_1}/\hbar$ and $k_2 = \sqrt{2mE_2}/\hbar$,

$$u''_{k_1}(r) - U(r)u_{k_1}(r) + k_1^2 u_{k_1}(r) = 0,$$
$$u''_{k_2}(r) - U(r)u_{k_2}(r) + k_2^2 u_{k_2}(r) = 0.$$

- Next, we multiply the first equation by u_{k_2} and the second by u_{k_1} and take their difference,

$$u''_{k_1}(r)u_{k_2}(r) - u_{k_1}(r)u''_{k_2}(r) = (k_2^2 - k_1^2)u_{k_1}(r)u_{k_2}(r).$$

- We may write the LHS as

$$u''_{k_1}(r)u_{k_2}(r) - u_{k_1}(r)u''_{k_2}(r) = \frac{d}{dr}\left[u'_{k_1}(r)u_{k_2}(r) - u'_{k_2}(r)u_{k_1}(r)\right]$$

The effective range

- Now we integrate from 0 to R,

$$\left[u'_{k_2}(r)u_{k_1}(r) - u'_{k_1}(r)u_{k_2}(r)\right]_0^R = (k_2^2 - k_1^2)\int_0^R dr\, u_{k_1}(r)u_{k_2}(r)$$

- The integral converges since $A_0(r) = u_0(r)/r$ is finite at the origin ($u_0(0) = 0$ independently of the energy).
- Next, we repeat the same procedure for the free-particle ($V = 0$) radial equation with solutions denoted by $g_{k_1}(r)$ and $g_{k_2}(r)$. The result is the same if we replace u by g
- The free-particle solution is also given by

$$g(r) = \cot\delta_0(k)\sin(kr) + \cos(kr)$$

- Note that we do not require $g(0) = 0$

The effective range

- Finally, we take the difference between the results

$$\left[g'_{k_2}(r)g_{k_1}(r) - g'_{k_1}(r)g_{k_2}(r)\right]_0^R - \left[u'_{k_2}(r)u_{k_1}(r) - u'_{k_1}(r)u_{k_2}(r)\right]_0^R = (k_2^2 - k_1^2)\int_0^R dr\left[g_{k_1}(r)g_{k_2}(r) - u_{k_1}(r)u_{k_2}(r)\right]$$

- The radial solution, $u_0(r)/r$, is finite at $r = 0$, thus $u_0(0) = 0$.
- $g(r)$ and $u(r > R)$ are equal for $r \geq R$
- Then we are left with

$$g'_{k_2}(0)g_{k_1}(0) - g'_{k_1}(0)g_{k_2}(0) = (k_2^2 - k_1^2)\int_0^R dr\left[g_{k_1}(r)g_{k_2}(r) - u_{k_1}(r)u_{k_2}(r)\right]$$

The effective range

- Using $g(r) = \cot\delta_0(k)\sin(kr) + \cos(kr)$ in the RHS

$$k_2 \cot\delta_0(k_2) - k_1 \cot\delta_0(k_1) = (k_2^2 - k_1^2)\int_0^R dr\,[g_{k_1}(r)g_{k_2}(r) - u_{k_1}(r)u_{k_2}(r)]$$

- If we take the limit $k_1 \to 0$, we can write $k_1 \cot\delta_0(k_1)$ in terms of the scattering length

$$k\cot\delta_0(k) = -\frac{1}{a} + k^2\int_0^R dr\,[g_0(r)g_k(r) - u_0(r)u_k(r)]$$

- We define the next term $r_0/2$ as

$$r_0 \equiv \lim_{k\to 0}\rho(k) = 2\int_0^R dr\,[g_0^2(r) - u_0^2(r)]$$

- r_0 is called effective range

Shape-independent approximation

- The resultant expression is the shape-independent approximation

$$k \cot \delta_0(k) = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \mathcal{O}(k^4)$$

- We are describing the phase shift $\delta_0(k)$ without taking into account the microscopic parameters of the scattering potential

Bound states

- Let us rewrite the scattered wave function at $r \to \infty$ as

$$\psi(r,\theta) \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} \frac{(2l+1)}{2ik} P_l(\cos\theta) \left[S_l(k) \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right]$$

- For $l = 0$ and large distances, the radial wave function is proportional to

$$S_0(k) \frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}$$

Bound states

- For an arbitrary finite-ranged potential V, the radial solution at $r > R$ for a bound state ($E < 0$) obeys

$$u''(r) = -\frac{2mE}{\hbar^2}u(r) = \kappa^2 u(r), \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$$

- The solution can be written as

$$u(r > R) = \cancel{Ae^{\kappa r}}^{0} + Be^{-\kappa r}$$

- We conclude that the radial function for a bound state at large distances is

$$A(r) = \frac{u(r)}{r} \propto \frac{e^{-\kappa r}}{r} \text{ (large } r\text{)}.$$

Bound states

- Scattered solution

$$S_0(k)\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}$$

- Bound state solution

$$\frac{e^{-\kappa r}}{r}$$

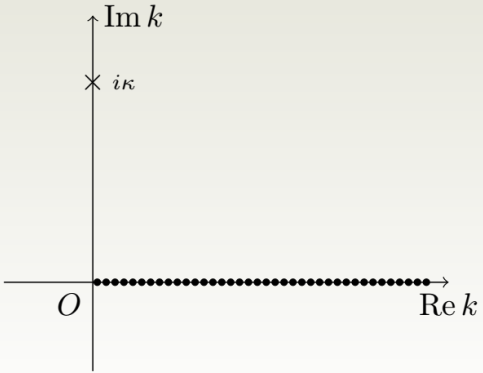
- By substituting $k \to i\kappa$, with k purely imaginary, we can connect the bound state with the scattered solution

$$\frac{e^{ikr}}{r} = \frac{e^{i(i\kappa)r}}{r} = \frac{e^{-\kappa r}}{r}$$

- $S_0(k)$ controls the ratio of the outgoing to the incoming wave
- In the bound state case, we have only the outgoing spherical wave, thus $S_0(k) \to \infty$

Bound states

- $S_l(k) = 1 + 2ikf_l(k) = e^{2i\delta_l(k)}$ is a complex function
- $S_0(k) \to \infty$ by substituting $k \to i\kappa$ means it has a pole at $k = i\kappa$



Bound states

- In terms of the s-wave scattering amplitude $f_0(k)$

$$f_0(k) = \frac{1}{k \cot \delta_0 - ik} = \frac{1}{-1/a - ik}$$

- We write $S_0(k)$ as

$$S_0(k) = 1 + 2ikf_0(k) = \frac{-k - i/a}{k - i/a}$$

- This expression has a pole at $k = i\kappa$ if we identify

$$\kappa = \frac{1}{a}$$

- In the zero-energy limit, the energy of a bound state and the scattering length are connected simply by

$$E = \frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{\hbar^2}{2ma^2}$$

- A single parameter originated from the potential determines the bound-state energy

Two-body scattering

- So far, we considered only the problem of a single particle being scattered by a finite-ranged potential $V(r)$ located at $r = 0$.
- With a few modifications, we can use the results we obtained to describe two particles interacting through a pairwise potential which depends only on their spatial separation r
- The Hamiltonian of a two-body system is separable in the center of mass (CM) and relative coordinates

$$H = -\frac{\hbar^2}{2m_1}\nabla^2_{\mathbf{r}_1} - \frac{\hbar^2}{2m_2}\nabla^2_{\mathbf{r}_2} + V(\mathbf{r}_1 - \mathbf{r}_2)$$

Two-body scattering

- We define the CM and relative coordinates

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{M} \quad \text{and} \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

- H is now separable

$$\begin{aligned} H &= H_{\text{CM}} + H_r, \\ H_{\text{CM}} &= -\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}}, \\ H_r &= -\frac{\hbar^2}{2m_r}\nabla^2_{\mathbf{r}} + V(r) \end{aligned}$$

- $m_r = m_1 m_2/(m_1 + m_2)$ is the reduced mass

Applications

1. Spherically symmetric finite well
   - Analytical calculation of the s-wave scattering wave function
     1. Scattering states ($E > 0$)
     2. Bound states ($E < 0$)
   - Calculation of the scattering length and effective range
2. Zero-range and finite-range approximations
   - Estimating bound state energies using the scattering length and effective range expansions

Spherically-symmetric finite well

- One way of defining the spherical well is

$$V_{\mathrm{sw}}(r) = \begin{cases} -V_0 & \text{for } r < R, \\ 0 & \text{for } r > R. \end{cases}$$

- V_0 has units of [energy]
- It will be clear in the numerical section that it is useful to redefine the potential as

$$V(r) = \begin{cases} -v_0 \dfrac{\hbar^2}{m_r R^2} & \text{for } r < R, \\ 0 & \text{for } r > R. \end{cases}$$

- v_0 is a dimensionless parameter related to the depth
- R is the potential range

Spherically-symmetric finite well ($E > 0$)

- Potential

$$V(r) = \begin{cases} -v_0 \dfrac{\hbar^2}{m_r R^2} & \text{for } r < R, \\ 0 & \text{for } r > R. \end{cases}$$

- $E > 0$ case

$$\left(\frac{d^2}{dr^2} - \frac{2m_r}{\hbar^2} V(r) + \frac{2m_r}{\hbar^2} E \right) u(r) = 0$$

→ Explicit forms for $r < R$ and $r > R$

$$\begin{aligned} u''(r) + \left(k_0^2 + k^2\right) u(r) &= 0 && \text{for } r < R, \\ u''(r) + k^2 u(r) &= 0 && \text{for } r > R, \end{aligned}$$

→ $k^2 \equiv 2m_r E/\hbar^2$ and $k_0^2 \equiv 2v_0/R^2$

Spherically-symmetric finite well ($E > 0$)

→ If $r < R$

$$u(r) = A \sin\left(\sqrt{k^2 + k_0^2}\, r\right) + B \cos\left(\sqrt{k^2 + k_0^2}\, r\right)$$

- Since $u_0(0) = 0$, we set $B = 0$

→ If $r < R$

$$u_0(r) = \cot \delta_0(k) \sin(kr) + \cos(kr)$$

→ Hence, the solution is of the form

$$u(r) = \begin{cases} A \sin\left(\sqrt{k^2 + k_0^2}\, r\right) & \text{for } r < R, \\ \cot \delta_0(k) \sin(kr) + \cos(kr) & \text{for } r > R. \end{cases}$$

Spherically-symmetric finite well ($E > 0$)

- Logarithmic derivative at $r = R^-$ and $r = R^+$

$$\left[r \frac{u'(r)}{u(r)} \right]_{r=R^-} = \left[r \frac{u'(r)}{u(r)} \right]_{r=R^+}$$

$$\frac{\sqrt{k^2 + k_0^2} \cos\left(\sqrt{k^2 + k_0^2}\, R \right)}{\sin\left(\sqrt{k^2 + k_0^2}\, R \right)} = \frac{k \cot \delta_0(k) \cos(kR) - k \sin(kR)}{\cot \delta_0(k) \sin(kR) + \cos(kR)}$$

- Solving for the phase shift $\delta_0(k)$ **without any approximation**

$$\delta_0(k) = -kR + \arctan \left[\frac{k \tan\left(\sqrt{k^2 + k_0^2}\, R \right)}{\sqrt{k^2 + k_0^2}} \right]$$

Spherically-symmetric finite well ($E > 0$)

- Scattering length
  - To calculate the scattering length a, we need to take the $k \to 0$ limit
  - Rearrange the log derivative so that we collect factors of $k \cot \delta_0(k)$
  - Keep track of the orders employed in the approximation

$$\begin{aligned} \cos(kR) &= 1 + \mathcal{O}(k^2) \\ \sin(kR) &= kR + \mathcal{O}(k^3) \end{aligned}$$

- Repeating last slides' equation:

$$\frac{\sqrt{k^2 + k_0^2}\cos\left(\sqrt{k^2 + k_0^2}\,R\right)}{\sin\left(\sqrt{k^2 + k_0^2}\,R\right)} = \frac{k\cot\delta_0(k)\cos(kR) - k\sin(kR)}{\cot\delta_0(k)\sin(kR) + \cos(kR)}$$

- Taking the $k \to 0$ limit:

$$\sqrt{k_0^2}\cot\left(\sqrt{k_0^2}\,R\right) = \frac{-1/a}{-R/a + 1}$$

Spherically-symmetric finite well ($E > 0$)

- Solving for a:

$$a = R - \frac{\tan\left(\sqrt{k_0^2}R\right)}{\sqrt{k_0^2}}$$

- The result is:

$$\boxed{a = R - \frac{\tan\left(\sqrt{k_0^2}R\right)}{\sqrt{k_0^2}} = R\left(1 - \frac{\tan\left(\sqrt{2v_0}\right)}{\sqrt{2v_0}}\right)}$$

- It is clear that a depends only on the parameters of the potential, its depth v_0 and range R
- Note that $\tan(x) \to \infty$ for $x = \frac{\pi}{2} + n\pi, \quad n = 0, \pm 1, \pm 2, ...$
- So the first divergence ($n = 0$) of a appears at

$$v_0 = \frac{\pi^2}{8}$$

Spherically-symmetric finite well ($E < 0$)

- $E < 0$ case
- Repeat the same procedure or $\boxed{k = i\kappa} \rightarrow E = \hbar^2 k^2/2m_r = -\hbar^2\kappa^2/2m_r$

$$\left(\frac{d^2}{dr^2} - \frac{2m_r}{\hbar^2}V(r) - \frac{2m_r}{\hbar^2}|E|\right)u(r) = 0$$

- Solution for $u(r)$

$$u(r) = \begin{cases} A' \sin\left(\sqrt{k_0^2 - \kappa^2}\, r\right) & \text{for } r < R, \\ B' e^{-\kappa r} & \text{for } r > R \end{cases}$$

- Match the logarithmic derivatives at $r = R$,

$$\frac{\sqrt{k_0^2 - \kappa^2}\cos\left(\sqrt{k_0^2 - \kappa^2}\, R\right)}{\sin\left(\sqrt{k_0^2 - \kappa^2}\, R\right)} = \frac{-\kappa e^{-\kappa R}}{e^{-\kappa R}}$$

Spherically-symmetric finite well ($E < 0$)

- After some manipulations,

$$\tan\left(\sqrt{k_0^2 - \kappa^2}\, R\right) + \frac{\sqrt{k_0^2 - \kappa^2}}{\kappa} = 0$$

- This is a transcendental equation that shows where the bound-state energies are located
- Note that the term $\sqrt{k_0^2 - \kappa^2}/\kappa$ is always positive
- $\tan\left(\sqrt{k_0^2 - \kappa^2}\, R\right)$ must be negative if we want the equation to have solution(s). That is to say:

$$\frac{\pi}{2} + n\pi < \sqrt{k_0^2 - \kappa^2}\, R < \pi + n\pi, \quad n = 0, 1, 2, ...$$

Spherically-symmetric finite well ($E < 0$)

- The first bound state is $n = 0$. Thus

$$\frac{\pi}{2R} < \sqrt{k_0^2 - \kappa^2} < \frac{\pi}{R}$$

- $k_0 > \sqrt{k_0^2 - \kappa^2}$
- Since $k_0 = \sqrt{2v_0}/R$, we have

$$v_0 > \frac{\pi^2}{8}$$

- This result shows that there are no bound states if v_0 is not above a certain threshold value
- This is the same threshold value that makes $|a| \to \infty$
- The conclusion is that the scattering length diverges when a bound state appears

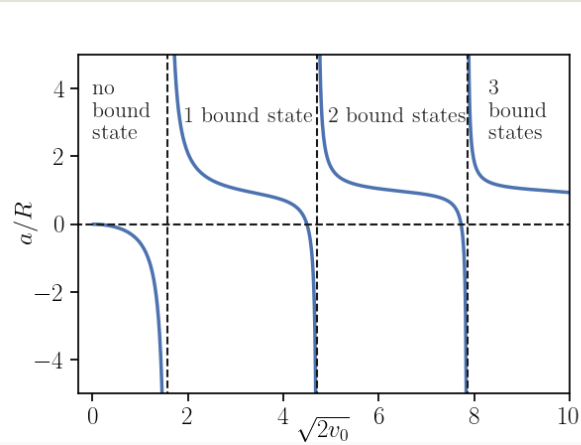
Spherically-symmetric well - bound states and scattering length

$$a = R\left(1 - \frac{\tan\left(\sqrt{2v_0}\right)}{\sqrt{2v_0}}\right)$$

- a diverges for:

$$\sqrt{2v_0} = \pi/2 + n\pi \qquad (n = 0, 1, 2, ...)$$

- This coincides with the location of the bound states



Spherically-symmetric finite well - effective range

- First, we need to determine the normalization constant of the scattering solution

$$u(r) = \begin{cases} A \sin\left(\sqrt{k^2 + k_0^2}\, r\right) & \text{for } r < R, \\ \cot\delta_0(k) \sin(kr) + \cos(kr) & \text{for } r > R \end{cases}$$

- To determine the constant A, we impose the continuity of $u(r)$ at $r = R$

$$A = \frac{\cot\delta_0(k) \sin(kR) + \cos(kR)}{\sin\left(\sqrt{k^2 + k_0^2} R\right)}$$

Spherically-symmetric finite well - effective range

- The normalized solution is written as

$$u(r) = \begin{cases} \frac{\cot\delta_0(k)\sin(kR)+\cos(kR)}{\sin(\sqrt{k^2+k_0^2}R)}\sin\left(\sqrt{k^2+k_0^2}\,r\right) & \text{for } r < R, \\ \cot\delta_0(k)\sin(kr)+\cos(kr) & \text{for } r > R. \end{cases}$$

- The effective range is defined in the $k \to 0$ limit of $u(r)$:

$$\lim_{k\to 0} u(r) = \begin{cases} \frac{(1-R/a)}{\sin(k_0R)}\sin(k_0r) & \text{for } r < R, \\ 1 - r/a & \text{for } r > R. \end{cases}$$

Spherically-symmetric finite well - effective range

- The effective range is given by the integral

$$r_0 = 2\int_0^R dr\left[\left(1-\frac{r}{a}\right)^2 - \left(1-\frac{R}{a}\right)^2 \frac{\sin^2(k_0 r)}{\sin^2(k_0 R)}\right]$$

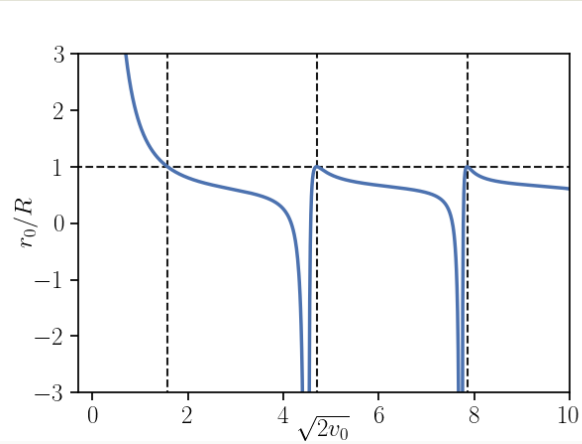
- Replacing a in favor of R and k_0:

$$\boxed{r_0 = R\left(1-\frac{1}{3}\left(\frac{k_0 R}{\tan(k_0 R)-k_0 R}\right)^2 + \frac{1}{k_0 R\tan(k_0 R)-(k_0 R)^2}\right)}$$

- This shows that r_0 also depends only on parameters of the potential

Spherically-symmetric finite well - effective range

$$r_0 = R\left(1 - \frac{1}{3}\left(\frac{k_0R}{\tan(k_0R) - k_0R}\right)^2 + \frac{1}{k_0R\tan(k_0R) - (k_0R)^2}\right)$$



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Zero-range and finite-range approximations

- The equation derived in the bound states slide allows us to estimate the bound state energy with the zero-range approximation $\kappa = 1/a$,

$$E_{zr} = -\frac{\hbar^2\kappa^2}{2m_r} = -\frac{\hbar^2}{2m_r a^2}$$

- To take the effective range into account, we write the s-wave scattering amplitude as

$$f_0(k) = \frac{1}{k\cot\delta_0(k) - ik} = \frac{1}{-1/a + r_0k^2/2 - ik}$$

- And $S_0(k)$ as

$$S_0(k) = 1 + 2ikf_0(k) = \frac{-i/a - k + ir_0k^2/2}{-i/a + k + ir_0k^2/2}$$

- Making $k \to i\kappa$

$$S_0(k) = \frac{-1/a - \kappa - r_0\kappa^2/2}{-1/a + \kappa - r_0\kappa^2/2}$$

Zero-range and finite-range approximations

- Now we can identify the bound state as pole in the S-matrix by solving

$$-1/a + \kappa - r_0\kappa^2/2 = 0$$

- which yields the solution

$$\kappa = \frac{1}{r_0}\left(1 \mp \sqrt{1 - \frac{2r_0}{a}}\right)$$

- Now choosing the appropriate root to compute the bound state energy

$$E_{fr} = -\frac{\hbar^2\kappa^2}{2m_r} = -\frac{\hbar^2}{2m_r r_0^2}\left(1 - \sqrt{1 - \frac{2r_0}{a}}\right)^2$$

Zero-range and finite-range approximations

- Example: Helium dimer
  - $E_d = -1.62$ mK (found solving the full Schrödinger equation), $a = 90.4$ Å, $r_0 = 8.0$ Å

$\rightarrow$ Zero-range approximation

$$\frac{E_{zr}}{k_b} = -\frac{\hbar^2}{k_b \times 2m_r a^2} = -1.48 \text{ mK} \qquad (92\%)$$

$\rightarrow$ Finite-range approximation

$$\frac{E_{fr}}{k_b} = -\frac{\hbar^2}{k_b \times 2m_r r_0^2}\left(1 - \sqrt{1 - \frac{2r_0}{a}}\right)^2 = -1.63 \text{ mK} \qquad (101\%)$$

- Both the zero- and finite-range results successfully describe the physical system because $kR \sim 0.1$

Zero-range and finite-range approximations

- Example: Deuteron
  - $E_d c^2 = -2.224$ MeV, $a = 5.4112$ fm, $r_0 = 1.7436$ fm.

→ Zero-range approximation

$$E_{zr} c^2 = -\frac{\hbar^2 c^2}{2 m_r a^2} = -1.416 \text{ MeV} \qquad (64\%)$$

→ Finite-range approximation

$$E_{fr} c^2 = -\frac{\hbar^2 c^2}{2 m_r r_0^2} \left(1 - \sqrt{1 - \frac{2 r_0}{a}} \right)^2 = -2.223 \text{ MeV} \qquad (100\%)$$

- The range of the potential needed to be taken into account because $kR \sim 0.4$
- We should emphasize that the scales are very different in both examples
- ^{4}He dimer: spatial scale of Å (10^{-10} m) and the energy is of the order of 10^{-7} eV
- Deuteron: the lengths are in the femtometer (10^{-15} m) scale, while the energy is of a few MeV (10^6 eV)
- This exemplifies how universal are these low-energy scattering results

Numerical Procedure

- Analytical expressions for the low-energy scattering parameters are only available for a few potentials
- Even in those cases, the calculations may be cumbersome, as we saw for the spherical well
- In general, we need to calculate a and r_0 numerically
- We will describe two methods to solve the Schrödinger equation numerically
  1. Second-order central difference
  2. Numerov's method

Numerical Procedure

- We wish to compute the quantities a and r_0
- To do so, we need to compute the radial solution inside and outside the potential range
  - $u_0(r < R)$: needs to be computed numerically
  - $u_0(r > R) = 1 - r/a$

Second-order central difference

- Consider the function $u(r)$ on a discrete set of points $r_i = i\Delta r$, $i = 0, 1, 2..., N$ and $\Delta r \ll 1$
- Let us take two Taylor expansions of $u(r)$ around the points $r \pm \Delta r$

$$u(r + \Delta r) = u(r) + (\Delta r)u'(r) + \frac{(\Delta r)^2}{2}u''(r) + \frac{(\Delta r)^3}{6}u'''(r) + \cdots,$$

$$u(r - \Delta r) = u(r) - (\Delta r)u'(r) + \frac{(\Delta r)^2}{2}u''(r) - \frac{(\Delta r)^3}{6}u'''(r) + \cdots$$

- The difference of the two Taylor expansions yields an expression for the first derivative, while their sum results in the second derivative

$$\left.\frac{du}{dr}\right|_{r=r_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta r} + \mathcal{O}[(\Delta r)^3]$$

$$\left.\frac{d^2u}{dr^2}\right|_{r=r_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta r)^2} + \mathcal{O}[(\Delta r)^4]$$

Second-order central difference

- We want to solve the zero-energy Schrödinger equation inside the potential range

$$\left(\frac{d^2}{dr^2} - \frac{2m_r}{\hbar^2}V(r)\right) u_0^{(k=0)}(r) = 0$$

$$\left.\frac{d^2u}{dr^2}\right|_{r=r_i} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta r)^2}$$

- Substituting the central difference second derivative into $u''(r)$

$$\boxed{u_{i+1} = 2u_i - u_{i-1} + \frac{2m_r(\Delta r)^2}{\hbar^2}V(r_i)u_i}$$

Second-order central difference

$$\boxed{u_{i+1} = 2u_i - u_{i-1} + \frac{2m_r(\Delta r)^2}{\hbar^2} V(r_i)u_i}$$

- If we know the value of the radial solution for two consecutive points, r_{i-1} and r_i, we can calculate the value for the next point u_{i+1}
  - $\rightarrow$ $u(0) = 0$
  - $\rightarrow$ $u(\Delta r) = 1$
- This choice allows us to find a solution without worrying about the normalization
- Algorithm:
  1. Set $u_0 = 0$, $u_1 = 1$, and $i = 1$
  2. Compute u_{i+1}
  3. If $r_i \geqslant R + \Delta r$, stop. Else, increment i by one
  4. Go to step 2

Numerov's method

- The second-order central difference is one possible discretization for a numerical second derivative
- There are other alternatives if we want to improve the precision of our algorithm
- Numerov's method is a numerical technique capable of solving differential equations of second order when the first-order term is not present:

$$\frac{d^2y}{dx^2} = -\xi(x)y(x) + s(x)$$

- The s-wave zero-energy radial equation is of this form, with $y \to u$, $x \to r$, $s = 0$, and

$$\xi(r) = -\frac{2m_r}{\hbar^2}V(r)$$

Numerov's method

- The method provides a solution of the form

$$y_{i+1} = \frac{1}{\left(1 + \frac{(\Delta x)^2}{12}\xi_{i+1}\right)}\left\{2y_i\left(1 - \frac{5(\Delta x)^2}{12}\xi_i\right) - y_{i-1}\left(1 + \frac{(\Delta x)^2}{12}\xi_{i-1}\right) + \frac{(\Delta x)^2}{12}(s_{i+1} + 10s_i + s_{i-1})\right\} + \mathcal{O}[(\Delta x)^6]$$

- The algorithm is mostly unchanged if we use Numerov's method instead of the second-order central difference

Dimensionless quantities

- Schrödinger's equation contains relatively small quantities
  - → $\hbar \sim 10^{-34}$ J s (or $\sim 10^{-15}$ eV s)
  - → Typical masses, length, and energy scales are also small
- We wish to make Schrödinger's equation dimensionless
- Instead of this

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{m_r}{\hbar^2}E + \frac{m_r}{\hbar^2}V(r)\right) u_0(r) = 0$$

- we want to solve this

$$\left(-\frac{1}{2}\frac{d^2}{d\bar{r}^2} - \bar{E} + \bar{V}(\bar{r})\right) \bar{u}(\bar{r}) = 0$$

- "$\hbar = m_r = 1$"

Dimensionless quantities

- First, we choose a length scale ℓ
  - $\rightarrow$ The convenient value of ℓ depends on the system under study; for atomic physics, it may be 1 Å; for nuclear physics, we may use 1 fm or any other length scale that makes sense for a particular problem
- Then the dimensionless scaled distance is

$$\bar{r} = \frac{r}{\ell}$$

- The radial function $u(r)$ has units of [length]$^{-1/2}$ (remember that $\int dr|u(r)|^2 = 1$)

$$\bar{u}(\bar{r}) = \frac{u(r)}{\ell^{-1/2}}$$

Dimensionless quantities

- The second derivative becomes

$$\frac{d^2}{dr^2} = \frac{1}{\ell^2}\frac{d^2}{d\bar{r}^2}$$

- Going back to the equation:

$$-\frac{\hbar^2}{2m_r\ell^2}\frac{d^2\bar{u}}{d\bar{r}^2} + V(\bar{r})\bar{u} = E\bar{u}$$

- We can also define an energy scale

$$\epsilon = \frac{\hbar^2}{m_r\ell^2}$$

- And now we define the dimensionless energy and potential

$$\bar{E} = \frac{E}{\epsilon}, \quad \bar{V} = \frac{V}{\epsilon}$$

- Finally

$$\boxed{-\frac{1}{2}\frac{d^2\bar{u}}{d\bar{r}^2} + \bar{V}(\bar{r})\bar{u} = \bar{E}\bar{u}}$$

Scattering length and effective range

- After following the numerical solution for $u_0(r)$, we're ready to compute the scattering length and the effective range
- Scattering length
  - → We recall that logarithmic derivative of the wave function outside the potential range is given by

$$\left.\frac{g_0'(r)}{g_0(r)}\right|_{r=R^+} = \frac{1}{R-a}$$

  - → This should be equal to the logarithmic derivative of $u_0(r)$ at $r = R^-$

$$\left.\frac{g_0'(r)}{g_0(r)}\right|_{r=R^+} = \frac{1}{R-a} = \left.\frac{u_0'(r)}{u_0(r)}\right|_{r=R^-}$$

  - → We already have $u(R)$ and $u(R \pm \Delta r)$. Thus the derivative may be computed as

$$u'_{\text{num}}(R) = \left.\frac{du(r)}{dr}\right|_{r=R} = \frac{u(R+\Delta r) - u(R-\Delta r)}{2\Delta r}$$

Scattering length and effective range

- Scattering length
  - → Now solving for a

$$\boxed{a = R - \frac{2\Delta r\, u(R)}{u(R+\Delta r) - u(R-\Delta r)}}$$

  - → This expression depends on the ratio of the radial solution, so we ignored the normalization
- Effective range
  - → On the other hand, the effective range assumes a particular normalization choice
  - → We multiply $u(r)$ by a constant C such that

$$C = \frac{g(R)}{u(R)} = \frac{(1 - R/a)}{u(R)}$$

  - → The effective range is found by computing the integral

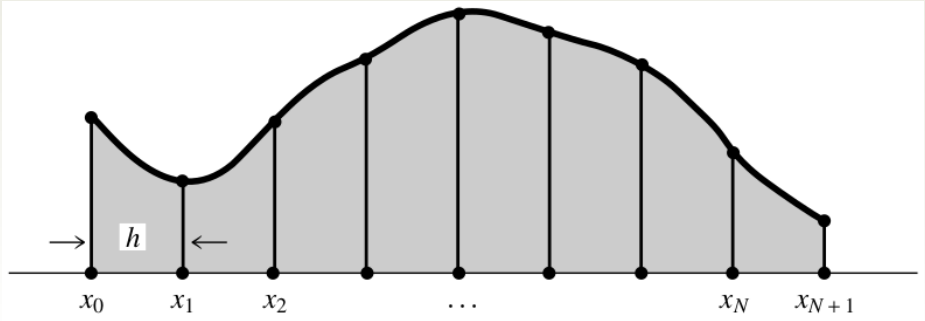
$$\boxed{r_0 = 2\int_0^R dr\,[g_0^2(r) - u_0^2(r)]}$$

Numerical integration

- The task is essentially to compute numerically an integral of the form

$$I = \int_{x_1}^{x_N} f(x)dx$$

- $f(x)$ is known only at a discrete set of equally spaced points, $f(x_i) \equiv f_i$, where $i = 1, 2, 3, ..., N$.



Numerical integration

- Trapezoidal rule:

$$\int_{x_1}^{x_2} f(x)dx = h\left[\frac{1}{2}f_1 + \frac{1}{2}f_2\right] + \mathcal{O}(h^3 f'')$$

- Using it $N-1$ times for the intervals: $(x_1, x_2), (x_2, x_3), \cdots, (x_{N-1}, x_N)$

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{2}f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2}f_N\right] + \mathcal{O}\left(\frac{(x_N - x_1)^3 f''}{N^2}\right)$$

Numerical integration

- Simpson's rule:

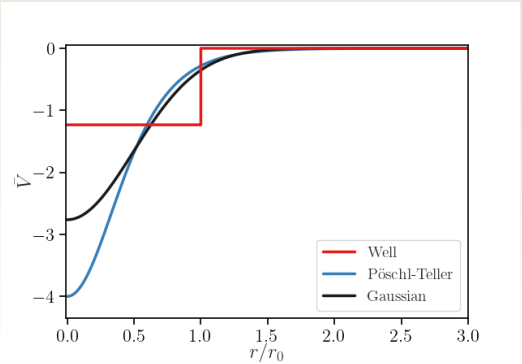
$$\int_{x_1}^{x_3} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{1}{3}f_3\right] + \mathcal{O}(h^5 f^{(4)})$$

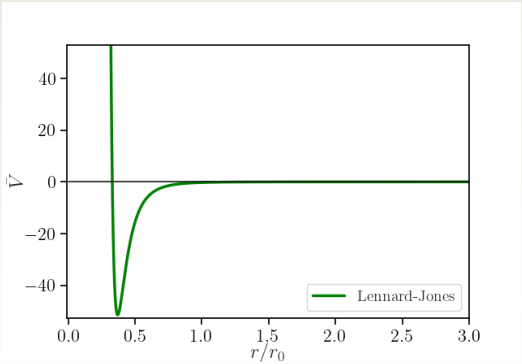
- Repeatedly:

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \cdots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right] + \mathcal{O}\left(\frac{(x_N - x_1)^5 f^{(4)}}{N^4}\right)$$

Examples

- We chose four potentials to illustrate the numerical procedure
  - → Spherical well
  - → Modified Pöschl-Teller
  - → Gaussian
  - → Lennard-Jones





Potentials - Spherical well

→ To make the comparison with other potentials easier, we redefine

$$V_{\text{sw}}(r) = \begin{cases} -v_{\text{sw}} \dfrac{\hbar^2 \mu_{\text{sw}}^2}{m_r}, & \text{for } r < R, \\ 0, & \text{for } r > R, \end{cases}$$

- v_{sw} is a dimensionless parameter related to the depth
- $\mu_{\text{sw}} = 1/R$

→ As we saw, $\epsilon = \frac{\hbar^2}{m_r \ell^2}$ makes Schrödinger's equation dimensionless

→ We can compare our numerical solutions with the analytical ones to check the correctness of the program

Potentials - Modified Pöschl-Teller (mPT)

$$V_{\mathrm{PT}}(r) = -v_{\mathrm{PT}} \frac{\hbar^2}{m_r} \frac{\mu_{\mathrm{PT}}^2}{\cosh^2(\mu_{\mathrm{PT}} r)}$$

- Very difficult analytical solution for the eigenfunctions
- There is an analytical expression for a in terms of the parameters of the potential

$$a\mu_{\mathrm{PT}} = \frac{\pi}{2} \cot\left(\frac{\pi\lambda}{2}\right) + \gamma + \Psi(\lambda),$$

- $v_{\mathrm{PT}} = \lambda(\lambda - 1)/2$, γ is the Euler-Mascheroni constant and Ψ is the digamma function
- The $|a| \to \infty$ case corresponds to $\lambda = 2$ ($\cot(\pi)$ diverges) or $\lambda = -1$ ($\Psi(-1)$ diverges), that is, $v_{\mathrm{PT}} = 1$
- For this particular case ($|a| \to \infty$), the s-wave zero-energy radial function takes a relatively simple form

$$u_0(r) = \frac{\tanh(\mu_{\mathrm{PT}}\, r)}{\tanh(\mu_{\mathrm{PT}}\, R)}$$

Potentials - mPT

- We can also calculate the effective range by performing the integral. In this case ($|a| \to \infty$), $g_0(r) = 1 - r/a = 1$, so that

$$r_0 = 2\int_0^R dr \left[1 - \frac{\tanh^2(\mu_{\rm PT} r)}{\tanh^2(\mu_{\rm PT} R)}\right] = 2\left[R - \frac{R}{\tanh^2(\mu_{\rm PT} R)} + \frac{1}{\mu_{\rm PT}\tanh(\mu_{\rm PT} R)}\right]$$

- Since $1/\mu_{\rm PT} \sim R$ and the $\tanh(x)$ function converges rapidly to 1 as we increase x, we may set $\tanh(\mu_{\rm PT} R) = 1$. Thus we have that $r_0 = 2/\mu_{\rm PT}$ for $v_{\rm PT} = 1$

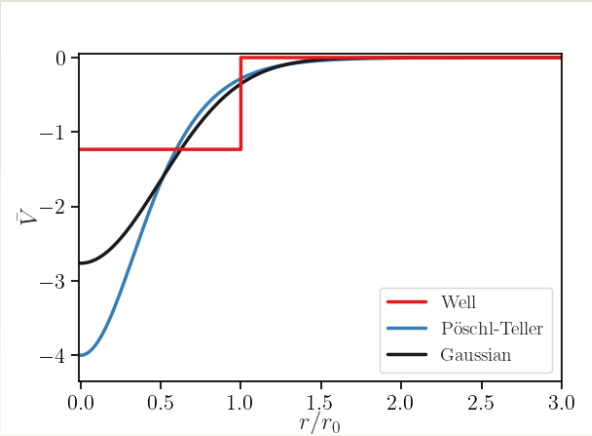
Potentials

- Spherical well
- Modified Pöschl-Teller

$$V_{\mathrm{PT}}(r) = -v_{\mathrm{PT}} \frac{\hbar^2}{m_r} \frac{\mu_{\mathrm{PT}}^2}{\cosh^2(\mu_{\mathrm{PT}} r)}$$

- Gaussian

$$V_{\mathrm{g}}(r) = -v_{\mathrm{g}} \frac{\hbar^2}{m_r} \mu_{\mathrm{g}}^2 e^{-r^2 \mu_{\mathrm{g}}^2}$$

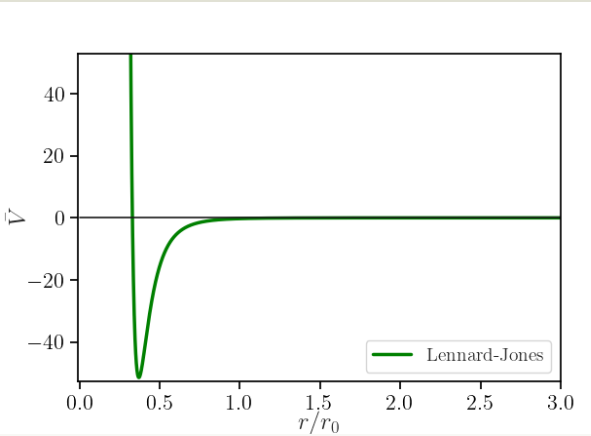


- The potential range R is not well defined for the mPT and the gaussian potentials
  → Look for a value of R such that the potential is negligible $|V(R)| \leqslant \varepsilon$

Potentials

- Lennard-Jones

$$V_{\mathrm{LJ}}(r) = \frac{\hbar^2}{m_r}\left[\frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}\right]$$



- Note that $V_{\mathrm{LJ}}(0)$ diverges and $V(\Delta r)$ is very large
  - We can safely set the boundary condition $u(0) = 0$ but computing $u(\Delta r)$ may lead to instabilities
  - Define a range $0 \leqslant r < r_{\mathrm{min}}$ where $u(r) = 0$ and start the integration at $r = r_{\mathrm{min}}$

Tuning the parameters

- The four potentials we presented have two parameters.
- Spherical well, mPT, Gaussian are purely attractive
  - one parameter is associated with the depth of the potential (v_{sw}, v_{PT}, and v_{g})
  - and another with its range (μ_{sw}, μ_{PT}, and μ_{g}).
- The LJ potential has a repulsive core and an attractive region
  - C_6 controls the attractive interaction
  - C_{12} controls the repulsive interaction
- Typically, the scattering length and effective range are known, and we want to tune the parameters of a particular potential to reproduce the desired a and r_0 values
- Since we want to match two values and have two free parameters, the correspondence is one-to-one (with the restriction of how many bound states we want)

Tuning the parameters

- To tune the parameters, we follow the following procedure
  1. Start with a guess (v_1, v_2).
  2. Compute a and r_0
  3. Keep v_2 fixed. Vary v_1 until a has the desired value. Increasing the depth of the potential will decrease the value of the scattering length (until it diverges and changes from $-\infty$ to $+\infty$).
  4. Keep v_1 fixed at the value found in step 3. Vary v_2 until r_0 has the desired value. Increasing the range of the potential will increase r_0.
  5. If a and r_0 match the desired values, stop. Else, go to step 3 and use the value of v_2 found in step 4.

Results

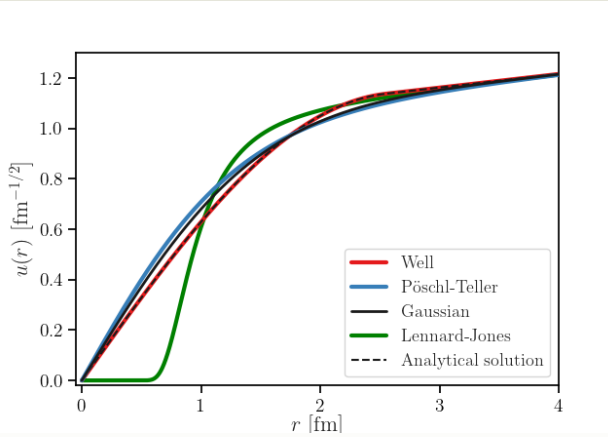
- We present 3 cases: $a < 0$, $|a| \to \infty$, and $a > 0$, which correspond to three very distinct physical situations.
  - $a < 0$
    - Example: neutron-neutron interaction ($a = -18.5$ fm , $r_0 = 2.7$ fm)
  - $|a| \to \infty$
    - Example: unitary Fermi gas
  - $a > 0$
    - Example: deuteron ($a = 5.4$ fm , $r_0 = 1.7$ fm)

System	a (fm)	r_0 (fm)
Neutron-neutron	-18.5	2.7
Unitarity	$\pm\infty$	1.0
Deuteron	5.4	1.7

Results

- $a < 0$

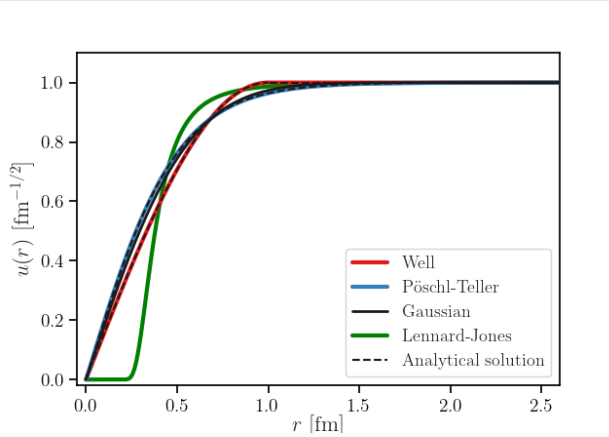
Potential	v	μ (fm^{-1})	a (fm)	r_0 (fm)
Neutron-neutron				
Well	1.1096	0.3918	−18.52	2.7
mPT	0.9071	0.7991	−18.51	2.7
Gaussian	1.2121	0.5672	−18.55	2.7



Results

- $|a| \to \infty$

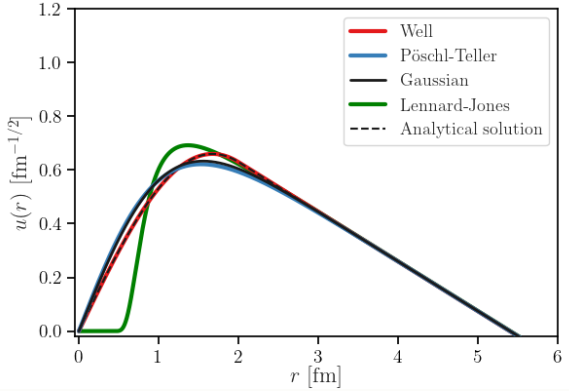
Potential	v	μ (fm^{-1})	a (fm)	r_0 (fm)
		Unitarity		
Well	1.2337	1.0000	$\sim -10^5$	1.0
mPT	1.0000	2.0000	$\sim 10^9$	1.0
Gaussian	1.3420	1.4349	$\sim -10^5$	1.0



Results

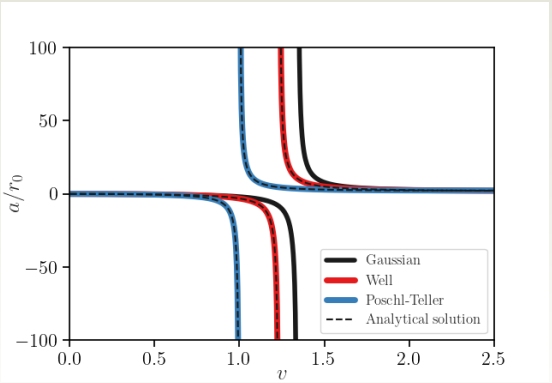
- $a > 0$

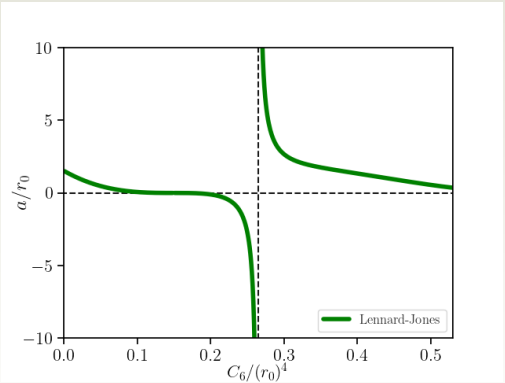
Potential	v	μ (fm^{-1})	a (fm)	r_0 (fm)
		Deuteron		
Well	1.2337	1.0000	$\sim -10^5$	1.0
mPT	1.0000	2.0000	$\sim 10^9$	1.0
Gaussian	1.3420	1.4349	$\sim -10^5$	1.0



Results

- Scattering length as a function of the strength of the attractive potential





Conclusions

- We presented quantum scattering theory fundamentals focusing on the low-energy limit
- In this context, we introduced two significant quantities: the scattering length and the effective range
- To illustrate how these two parameters behave in a concrete example, we derived analytical expressions for both in the case of the spherical well
- We also showed how the energy of a bound state could be calculated using zero- and finite-range expressions applied to a ^{4}He dimer and the deuteron
- We described a numerical procedure that can be used to compute the scattering length and effective range of any spherically symmetric finite-ranged two-body potential
  - Examples: spherical well, modified Pöschl-Teller, Gaussian, and Lennard-Jones potentials
- Now, you can extend what you learned to your choice of physical systems, and apply the method to other potentials