Low energy Nuclear Physics: Integral relations

Variational Bounds (1)

Two-body system: Bound states

$$(T+V-E_n)\Psi_n=0 \longrightarrow (-\frac{\hbar^2}{m}\nabla^2+V-E_n)\Psi_n(\mathbf{r})=0$$

For $E_n<0$ and $\ell=0$, $\Psi_n(\mathbf{r})=\phi_n(r)/\sqrt{4\pi}$

- numerical solution in a grid $\{r_i\}\to\phi_n(r_i),\mathcal{E}_n$

$$E_n=\frac{<\Psi_n|H|\Psi_n>}{<\Psi_n|\Psi_n>} \qquad |\frac{E_n-\mathcal{E}_n}{E_n}|\approx 10^{-7}$$

- expansion in a complete basis $\psi_k(r)\to\phi_n(r)=\sum_k^N A_k^n\psi_k(r)$

$$\sum_k^N<\psi_{k'}|H-\mathcal{E}|\psi_k>=0 \qquad \mathcal{E}_n\geq E_n\ \text{and, for}\ N\to\infty,\ \mathcal{E}_n\longrightarrow E_n$$

Variational Bounds (1)

Two-body system: Bound states

$$(T + V - E_n)\Psi_n = 0 \longrightarrow (-\frac{\hbar^2}{m}\nabla^2 + V - E_n)\Psi_n(\boldsymbol{r}) = 0$$

For $E_n < 0$ and $\ell = 0$, $\Psi_n(\boldsymbol{r}) = \phi_n(r)/\sqrt{4\pi}$

- numerical solution in a grid $\{r_i\} \rightarrow \phi_n(r_i), \mathcal{E}_n$

$$E_n = \frac{< \Psi_n|H|\Psi_n >}{< \Psi_n|\Psi_n >} \qquad |\frac{E_n - \mathcal{E}_n}{E_n}| \approx 10^{-7}$$

- expansion in a complete basis $\psi_k(r) \rightarrow \phi_n(r) = \sum_k^N A_k^n \psi_k(r)$

$$\sum_k^N < \psi_{k'}|H - \mathcal{E}|\psi_k >= 0 \qquad \mathcal{E}_n \geq E_n \text{ and, for } N \rightarrow \infty, \ \mathcal{E}_n \longrightarrow E_n$$

Variational Bounds (1)

Two-body system: Bound states

$$(T + V - E_n)\Psi_n = 0 \longrightarrow (-\frac{\hbar^2}{m}\nabla^2 + V - E_n)\Psi_n(\boldsymbol{r}) = 0$$

For $E_n < 0$ and $\ell = 0$, $\Psi_n(\boldsymbol{r}) = \phi_n(r)/\sqrt{4\pi}$

• numerical solution in a grid $\{r_i\} \to \phi_n(r_i), \mathcal{E}_n$

$$E_n = \frac{< \Psi_n|H|\Psi_n >}{< \Psi_n|\Psi_n >} \qquad |\frac{E_n - \mathcal{E}_n}{E_n}| \approx 10^{-7}$$

• expansion in a complete basis $\psi_k(r) \to \phi_n(r) = \sum_k^N A_k^n \psi_k(r)$

$$\sum_k^N < \psi_{k'}|H - \mathcal{E}|\psi_k >= 0 \qquad \mathcal{E}_n \geq E_n \text{ and, for } N \to \infty, \ \mathcal{E}_n \longrightarrow E_n$$

Integral relations for the phase-shift

Let us recall the asymptotic behavior of the wave function. For simplicity we consider $\ell = 0$, uncoupled channels, and not consider spin,sisopin degrees of freedom.

$$\Psi(r) = \frac{u(r)}{r}\frac{1}{4\pi} \longrightarrow \sqrt{\frac{k}{4\pi}}\left[A\frac{\sin kr}{kr} + B\frac{\cos kr}{kr}\right] = AF + BG$$

where we have defined

$$\begin{cases} F = \sqrt{\frac{k}{4\pi}}\frac{\sin kr}{kr} \\ \\ G = \sqrt{\frac{k}{4\pi}}\frac{\cos kr}{kr} \end{cases}$$

The asymptotic solutions verify the Wronskian

$$W(F,G) = \frac{m}{\hbar^2}\left[< F|H-E|G > - < G|H-E|F >\right] = 1$$

Demonstration

Explicitely the relation is

$$\frac{m}{\hbar^2}\left[\int F[-\frac{\hbar^2}{m}\nabla^2 + V - E]G\,d\vec{r} - \int G[-\frac{\hbar^2}{m}\nabla^2 + V - E]F\,d\vec{r}\right]$$

the terms in the potential V cancel and remains

$$-\int F[\nabla^2 + k^2]G\,d\vec{r} + \int G[\nabla^2 + k^2]F\,d\vec{r}$$

F is the regular solution of $(\nabla^2 + k^2)F = 0$. Instead for the irregular term $(\nabla^2 + k^2)G = -4\pi\delta(\vec{r})/\sqrt{4\pi k}$. Therefore the second term is zero and the first term reduced to

$$W(F, G) = 4\pi\frac{F(0)}{\sqrt{4\pi k}} = 1$$

Integral relations for the phase-shift

The asymptotic coefficients of the wave function $\Psi \rightarrow AF + BG$ are obtained from the following relations

$$B = W(F, \Psi) = \frac{m}{\hbar^2}\left[< F|H - E|\Psi > - < \Psi|H - E|F >\right]$$

$$A = W(\Psi, G) = \frac{m}{\hbar^2}\left[< \Psi|H - E|G > - < G|H - E|\Psi >\right]$$

Here I am using the Green's Theorem

$$\int_V (\Psi\nabla^2\Phi - \Phi\nabla^2\Psi)dV = \int_S (\Psi\frac{\partial\Phi}{\partial n} - \Phi\frac{\partial\Psi}{\partial n})dS$$

The derivative terms in the surface integral form the Wronskian

Integral relations for the phase-shift

The asymptotic coefficients of the wave function $\Psi \rightarrow AF + BG$ are obtained from the following relations

$$B = W(F,\Psi) = \frac{m}{\hbar^2}[< F|H-E|\Psi > - < \Psi|H-E|F >]$$

$$A = W(\Psi,G) = \frac{m}{\hbar^2}[< \Psi|H-E|G > - < G|H-E|\Psi >]$$

However, since the wave function verifies $(H-E)\Psi = 0$ we have

$$\begin{cases} B = -\frac{m}{\hbar^2} < \Psi|H-E|F > \\ \\ A = \frac{m}{\hbar^2} < \Psi|H-E|G > \end{cases}$$

and

$$\tan\delta = \frac{B}{A}$$

To be noticed that the integrals are short-range: the phase-shift is determined by the short-range part of the wave funtion!

Short-range character

Explicitly the integrals are

$$\begin{cases} B = -\frac{m}{k\hbar^2}\int_0^\infty \sin kr\, V(r)u(r)dr \\ A = \frac{m}{k\hbar^2}\int_0^\infty \cos kr\, V(r)u(r)dr + \frac{1}{k}\frac{u(r)}{r}\Big|_{r=0} \end{cases}$$

It is possible to introduced a regularized function $\widetilde{G} = f_\gamma G$, with

$$\widetilde{G} \xrightarrow{r\to 0} \text{regular} \qquad\qquad \widetilde{G} \xrightarrow{r\to\infty} G$$

For example: $\widetilde{G} = (1 - e^{-\gamma r})G$, which is regular at the origin. And the las integarls is now

$$A = \frac{m}{k\hbar^2}\int_0^\infty \cos kr\, V(r)u(r)dr + I_\gamma$$

with I_γ a short-range integral

Short-range character

I_γ contains all terms depending on γ, introduced by the factor $(1-e^{-\gamma r})$:

$$I_\gamma = -\frac{1}{\sqrt{k}}\int_0^\infty dr\left(\frac{m}{\hbar^2}V(r)\cos kr - \gamma^2\cos kr - 2\gamma k\sin kr\right)\mathrm{e}^{-\gamma r}u(r)$$

- Remarkably it does not depend on γ
- We identify $I_\gamma = \frac{1}{k}\frac{u(r)}{r}|_{r=0}$.
- This equality can be verified with the same relative accuracy obtained for $\tan\delta$ provided that the regularization of G is done inside the interaction region.

Variational Bounds (2)

Two-body system: Scattering states

$$(T+V-E)\Psi_k = 0 \longrightarrow (-\frac{\hbar^2}{m}\nabla^2 + V - E)\Psi_k(\mathbf{r}) = 0$$

For $k^2 = \frac{m}{\hbar^2}E$ and $\ell = 0$, $\Psi_k(\mathbf{r}) = \phi_k(r)/\sqrt{4\pi}$

Asymptotic behavior $\phi(r \to \infty) \longrightarrow \sqrt{k}\left[A\frac{\sin(kr)}{kr} + B\frac{\cos(kr)}{kr}\right]$

- numerical solution in a grid $\{r_i\} \to \phi_k(r_i), A, B$ $\quad \tan\delta = B/A$

- the following integral relations are verified

$$\left.\begin{array}{l} -\frac{m}{\hbar^2} < \Psi_k|H-E|F >= B \quad \text{with} \quad F = \sqrt{\frac{k}{4\pi}}\frac{\sin(kr)}{kr} \\ \frac{m}{\hbar^2} < \Psi_k|H-E|G >= A \quad \text{with} \quad G = \sqrt{\frac{k}{4\pi}}\frac{\cos(kr)}{kr} \end{array}\right\} \tan\delta = \frac{B}{A}$$

$$\left|\frac{\tan\delta - \tan\delta}{\tan\delta}\right| \approx 10^{-7}$$

Variational Bounds (2)

Two-body system: Scattering states

$$(T+V-E)\Psi_k = 0 \longrightarrow \left(-\frac{\hbar^2}{m}\nabla^2 + V - E\right)\Psi_k(\mathbf{r}) = 0$$

For $k^2 = \frac{m}{\hbar^2}E$ and $\ell = 0$, $\Psi_k(\mathbf{r}) = \phi_k(r)/\sqrt{4\pi}$

Asymptotic behavior $\phi(r \to \infty) \longrightarrow \sqrt{k}\left[A\frac{\sin(kr)}{kr} + B\frac{\cos(kr)}{kr}\right]$

- numerical solution in a grid $\{r_i\} \to \phi_k(r_i), A, B$ $\qquad \tan\delta = B/A$

- the following integral relations are verified

$$\left.\begin{aligned} -\frac{m}{\hbar^2} < \Psi_k|H-E|F >= B \quad \text{with} \quad F = \sqrt{\frac{k}{4\pi}}\frac{\sin(kr)}{kr} \\ \frac{m}{\hbar^2} < \Psi_k|H-E|G >= A \quad \text{with} \quad G = \sqrt{\frac{k}{4\pi}}\frac{\cos(kr)}{kr} \end{aligned}\right\} \tan\delta = \frac{B}{A}$$

$$\left|\frac{\tan\delta - \tan\delta}{\tan\delta}\right| \approx 10^{-7}$$

Variational Bounds (2)

Two-body system: Scattering states

$$(T+V-E)\Psi_k=0 \longrightarrow (-\frac{\hbar^2}{m}\nabla^2+V-E)\Psi_k(\boldsymbol{r})=0$$

For $k^2=\frac{m}{\hbar^2}E$ and $\ell=0$, $\Psi_k(\boldsymbol{r})=\phi_k(r)/\sqrt{4\pi}$

Asymptotic behavior $\phi(r\to\infty)\longrightarrow\sqrt{k}\left[A\frac{\sin(kr)}{kr}+B\frac{\cos(kr)}{kr}\right]$

- numerical solution in a grid $\{r_i\}\to\phi_k(r_i), A, B$ $\qquad \tan\delta=B/A$

- the following integral relations are verified

$$\left.\begin{array}{lll} -\frac{m}{\hbar^2}<\Psi_k|H-E|F>=B & \text{with} & F=\sqrt{\frac{k}{4\pi}}\frac{\sin(kr)}{kr} \\ \frac{m}{\hbar^2}<\Psi_k|H-E|G>=A & \text{with} & G=\sqrt{\frac{k}{4\pi}}\frac{\cos(kr)}{kr} \end{array}\right\}\tan\delta=\frac{B}{A}$$

$$\left|\frac{\tan\delta-\tan\delta}{\tan\delta}\right|\approx 10^{-7}$$

Variational character

To be noticed that the phase-shift

$$\tan \delta = \frac{B}{A}$$

is independent of the regularization factor if $(H - E)\Psi = 0$.
Moreover, since $(H - E)F$ and $(H - E)G \to 0$ as $r \to \infty$. It is sufficient that $(H - E)\Psi = 0$ only inside the interaction region. This gives a variational character to the integral relations.

$$\begin{cases} B = -\frac{m}{\hbar^2} < \Psi_t | H - E | F > \\ \\ A = \frac{m}{\hbar^2} < \Psi_t | H - E | G > \end{cases}$$

For example we can choose $\Psi_t \to 0$ as $r \to \infty$, a square integrable function.

Variational Bounds (2) - continuation

The Rayleigh-Ritz Variational Principle

$$E = \frac{< \Psi_b | H | \Psi_b >}{< \Psi_b | \Psi_b >} \quad \text{or} \quad < \Psi_b | H - E | \Psi_b > = 0$$

the Kohn Variational Principle (for a single channel)

$$[\tan\delta] = \tan\delta - < \Psi_s | H - E | \Psi_s >$$

Expansion in a basis

Bound states: $\Psi_b = \sum_k C_k \psi_k(r) \qquad \psi_k(r \to \infty) \to 0$

Scattering states: $\Psi_s = \Psi_c + AF(r) + BG(r)$

with

$$\Psi_c = \sum_k D_k \psi_k(r)$$

Variational Bounds (2) - continuation

The Rayleigh-Ritz Variational Principle

$$E = \frac{< \Psi_b|H|\Psi_b >}{< \Psi_b|\Psi_b >} \quad \text{or} \quad < \Psi_b|H - E|\Psi_b >= 0$$

the Kohn Variational Principle (for a single channel)

$$[\tan\delta] = \tan\delta - < \Psi_s|H - E|\Psi_s >$$

Expansion in a basis

Bound states: $\Psi_b = \sum_k C_k \psi_k(r) \qquad \psi_k(r \to \infty) \to 0$

Scattering states: $\Psi_s = \Psi_c + AF(r) + BG(r)$

with

$$\Psi_c = \sum_k D_k \psi_k(r)$$

Variational Bounds (2) - continuation

The Rayleigh-Ritz Variational Principle

$$E = \frac{< \Psi_b | H | \Psi_b >}{< \Psi_b | \Psi_b >} \quad \text{or} \quad < \Psi_b | H - E | \Psi_b > = 0$$

the Kohn Variational Principle (for a single channel)

$$[\tan \delta] = \tan \delta - < \Psi_s | H - E | \Psi_s >$$

Expansion in a basis

Bound states: $\Psi_b = \sum_k C_k \psi_k(r) \qquad \psi_k(r \to \infty) \to 0$

Scattering states: $\Psi_s = \Psi_c + AF(r) + BG(r)$

with

$$\Psi_c = \sum_k D_k \psi_k(r)$$

$$\Psi_s = \Psi_c(r) + AF(r) + BG(r) \quad (\Psi_c \to 0 \text{ as } r \to \infty)$$

$$[\tan\delta] = \tan\delta - < (1/A)\Psi_s|H-E|(1/A)\Psi_s > \quad (\tan\delta = B/A)$$

The variation of the functional $\Delta[\tan\delta] = 0$ with respect to the linear parameters (D_k and $\tan\delta$) implies

a) $< \Psi_c|H-E|\Psi_s >= 0$

b) $1 - < G|H-E|(1/A)\Psi_s > - < (1/A)\Psi_s|H-E|G >= 0$

or $< G|H-E|(1/A)\Psi_s >= 0$

These two equations form a linear system from where the linear parameters D_k and $\tan\delta$ can be obtained.

using the Wronskian

$< F|H-E|G > - < G|H-E|F >= 1$

$< \Psi_s|H-E|G > - < G|H-E|\Psi_s >= A = < \Psi_s|H-E|G >$

$< F|H-E|\Psi_s > - < \Psi_s|H-E|F >= B^{1st}$

$$\Psi_s = \Psi_c(r) + AF(r) + BG(r) \quad (\Psi_c \to 0 \text{ as } r \to \infty)$$

$$[\tan\delta] = \tan\delta - < (1/A)\Psi_s|H-E|(1/A)\Psi_s > \quad (\tan\delta = B/A)$$

The variation of the functional $\Delta[\tan\delta] = 0$ with respect to the linear parameters (D_k and $\tan\delta$) implies

a) $< \Psi_c|H-E|\Psi_s >= 0$

b) $1 - < G|H-E|(1/A)\Psi_s > - < (1/A)\Psi_s|H-E|G >= 0$

or $< G|H-E|(1/A)\Psi_s >= 0$

These two equations form a linear system from where the linear parameters D_k and $\tan\delta$ can be obtained.

using the Wronskian

$$< F|H-E|G > - < G|H-E|F >= 1$$

$$< \Psi_s|H-E|G > - < G|H-E|\Psi_s >= A = < \Psi_s|H-E|G >$$

$$< F|H-E|\Psi_s > - < \Psi_s|H-E|F >= B^{1st}$$

The phase-shift obtained is considered first order $\rightarrow \tan\delta^{1st}$
The second order results:

$$[\tan\delta]^{2nd} = \tan\delta^{1st} - <(1/A)\Psi_s|H-E|(1/A)\Psi_s>$$

$$[\tan\delta]^{2nd} = \tan\delta^{1st} - <F|H-E|(1/A)\Psi_s>$$

multiplying by A the equation for $[\tan\delta]^{2nd}$

$$\begin{aligned} B^{2nd} &= -<\Psi_s|H-E|F> \\ A &= \;\; <\Psi_s|H-E|G> \\ [\tan\delta]^{2nd} &= \;\; B^{2nd}/A \end{aligned}$$

The Integral Relations for coupled channels

$$\begin{aligned} B^{2nd}_{ij} &= -<\Psi^s_i|H-E|F_j> \\ A_{ij} &= \;\; <\Psi^s_i|H-E|G_j> \\ [\mathcal{R}]^{2nd} &= \;\; A^{-1}B^{2nd} \qquad \text{(the eigenvalues of } \mathcal{R} \text{ are } \tan\delta) \end{aligned}$$

The phase-shift obtained is considered first order $\rightarrow \tan\delta^{1st}$
The second order results:

$$[\tan\delta]^{2nd} = \tan\delta^{1st} - < (1/A)\Psi_s | H - E | (1/A)\Psi_s >$$

$$[\tan\delta]^{2nd} = \tan\delta^{1st} - < F | H - E | (1/A)\Psi_s >$$

multiplying by A the equation for $[\tan\delta]^{2nd}$

$$B^{2nd} = - < \Psi_s | H - E | F >$$

$$A = < \Psi_s | H - E | G >$$

$$[\tan\delta]^{2nd} = B^{2nd}/A$$

The Integral Relations for coupled channels

$$B^{2nd}_{ij} = - < \Psi^s_i | H - E | F_j >$$

$$A_{ij} = < \Psi^s_i | H - E | G_j >$$

$$[\mathcal{R}]^{2nd} = A^{-1} B^{2nd} \qquad \text{(the eigenvalues of } \mathcal{R} \text{ are } \tan\delta)$$

Properties

- The integral relations have a variational character
- Direct applications of the KVP are made with $A = 1$
- However there are cases in which the explicit asymptotic behavior of Ψ_s in term of the coefficients A and B is not known
- The integrals converge even if $(H - E)\Psi_s \neq 0$ asymptotically
- If $(H - E)\Psi_s = 0$ in the interaction region, the result for $[\tan\delta]^{2nd}$ is exact, even if the asymptotic behavior of Ψ_s is not the physical one

The Integral Relations

$$B^{2nd} = - < \Psi_s | H - E | F >$$

$$A = < \Psi_s | H - E | G >$$

$$[\tan \delta]^{2nd} = B^{2nd} / A$$

The Integral Relations for coupled channels

$$B^{2nd}_{ij} = - < \Psi^s_i | H - E | F_j >$$

$$A_{ij} = < \Psi^s_i | H - E | G_j >$$

$$[\mathcal{R}]^{2nd} = A^{-1} B^{2nd}$$ (the eigenvalues of $\mathcal{R}$ are $\tan \delta$)

The Integral Relations

$$B^{2nd} = -<\Psi_s|H-E|F>$$
$$A = <\Psi_s|H-E|G>$$
$$[\tan\delta]^{2nd} = B^{2nd}/A$$

The Integral Relations for coupled channels

$$B_{ij}^{2nd} = -<\Psi_i^s|H-E|F_j>$$
$$A_{ij} = <\Psi_i^s|H-E|G_j>$$
$$[\mathcal{R}]^{2nd} = A^{-1}B^{2nd}$$ (the eigenvalues of $\mathcal{R}$ are $\tan\delta$)

Application for a central potential

Let us consider $\ell = 0$ and expand Ψ_t in a complete basis

$$\Psi_t(\vec{r}) = \frac{u(r)}{r}\frac{1}{\sqrt{4\pi}} = \frac{1}{\sqrt{4\pi}}\sum_m a_m \mathcal{L}_m^{(2)}(\beta r)e^{-\beta r/2}$$

with $\mathcal{L}_m^{(2)}(z)$ a Laguerre polynomial verifying

$$\int_0^\infty \mathcal{L}_m^{(2)}(z)\mathcal{L}_{m'}^{(2)}(z)e^{-z}r^2 dr = \delta_{mm'}$$

We transform the Hamiltonian in a matrix

$$H_{mm'} = \int_0^\infty \mathcal{L}_m^{(2)}(z)e^{-z/2}\left[-\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + V\right]\mathcal{L}_{m'}^{(2)}(z)e^{-z/2}r^2 dr$$

where $z = \beta r$ and β a nonlinear parameter

Variational bounds

The Rayleigh-Ritz principle establishes that the lowest eigenvalue of the hamiltonian matrix verifies

$$E_0^M \geq E_0, \quad \text{and} \quad E_0^M \stackrel{M\to\infty}{\longrightarrow} E_0$$

where M is the dimension of the bais and E_0 is the exact value of the ground state. Moreover the MacDonald-Hylleraas-Undheim theorem establishes that the same type of convergence results for the N lowest eigenvalues of the hamiltonian matrix

$$E_j^M \geq E_j, \quad \text{and} \quad E_j^M \stackrel{M\to\infty}{\longrightarrow} E_j$$

with E_j the exact excited state energy of the system.
In the case of positive energies, the spectrum represents a discretization of the continumm. In all cases the eigenvector

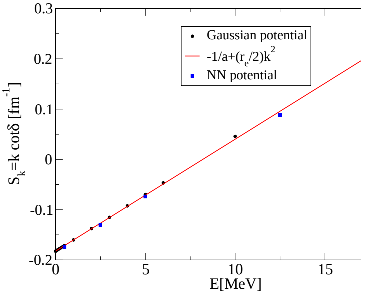
$$\Psi_j = \sum_m a_m^j \mathcal{L}_m^{(2)}(\beta r) e^{-\beta r/2}$$

is a representation of the wave function of the corresponding level.

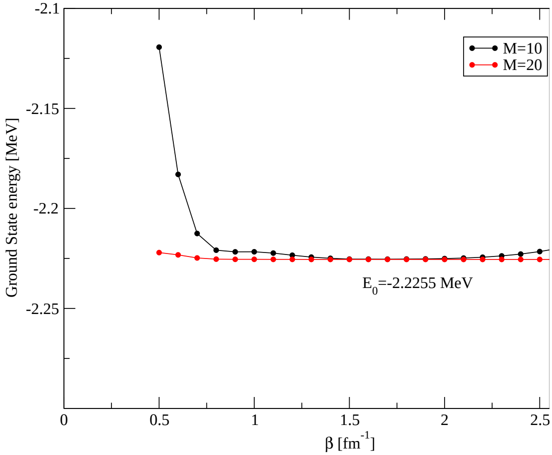
Example: Gaussian potential

$$V(r) = V_0 e^{-r^2/r_0^2}$$

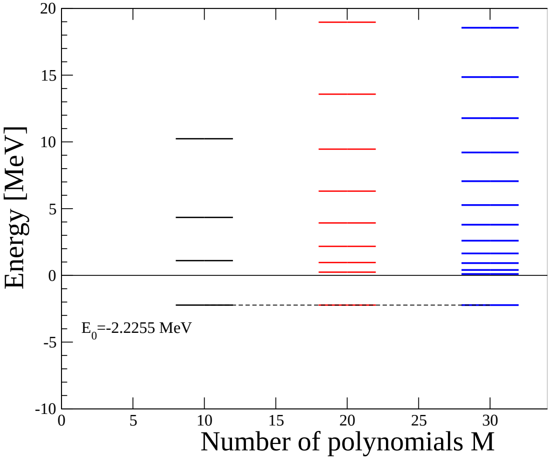
with $V_0 = -60.575\,\text{MeV}$ and $r_0 = 1.65\,\text{fm}$
This potential has one bound state $E_0 = -2.2255\,\text{MeV}$ and the low energy parameters are: $a = 5.480\,\text{fm}$ and $r_{eff} = 1.846\,\text{fm}$
very close to the experimental values. This potential is a low energy representation of the NN interaction ($\ell = 0, s = 1, t = 0$)



Ground state convergence



Positive energy discretization



Phases with the Integral Relation

Now we calculate the phases using the positive energy eigenvectors

$$\Psi_j^M = \sum_{m=0}^{M} a_m^j \mathcal{L}_m^{(2)}(\beta r) e^{-\beta r/2}$$

For each positive energy, the integral relations are:

$$\begin{cases} B_j^M = -\frac{m}{\hbar^2} < \Psi_j^M | H - E_j | F > \\ \\ A_j^M = \frac{m}{\hbar^2} < \Psi_j^M | H - E_j | G > \end{cases}$$

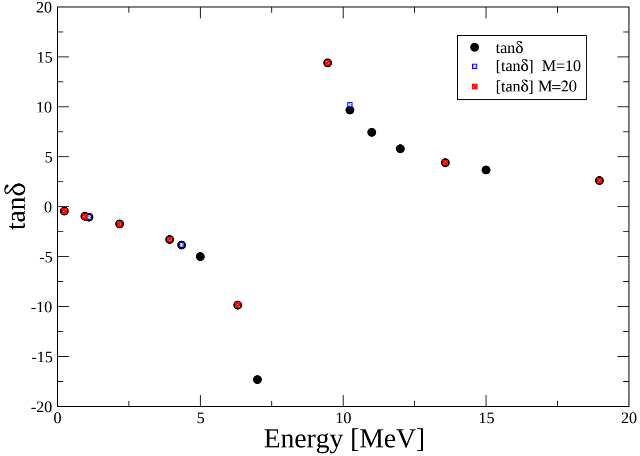
$$[\tan \delta_j^M]^{2nd} = \frac{B_j^M}{A_j^M}$$

where we give explicitely the second order character of the estimate and the dependence with the dimension of the basis M.

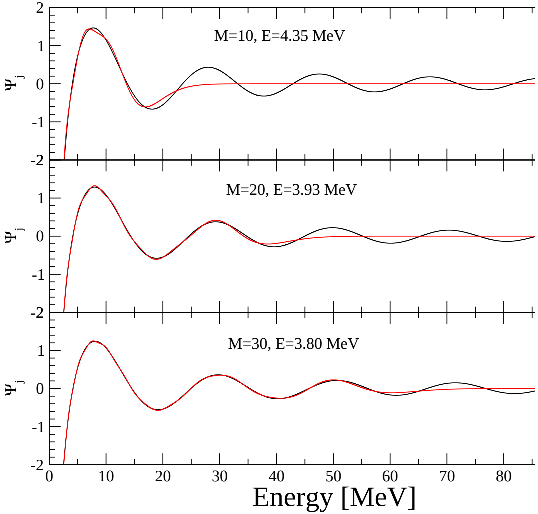
Convergence of the phases

M	10	20	30	40
E_0	-2.225322	-2.225505	-2.225506	-2.225506
E_1	0.536349	0.116356	0.048091	0.026008
$[\tan\delta_1]^{2^{nd}}$	-1.507280	-0.622242	-0.392005	-0.286479
$\tan\delta_1$	-1.522377	-0.621938	-0.392021	-0.286480
E_2	1.984580	0.449655	0.190019	0.103503
$[\tan\delta_2]^{2^{nd}}$	-5.919685	-1.353736	-0.812313	-0.584389
$\tan\delta_2$	-5.703495	-1.354691	-0.812270	-0.584388
E_3	4.512635	0.994433	0.423117	0.231645
$[\tan\delta_3]^{2^{nd}}$	13.998124	-2.451174	-1.302799	-0.908128
$\tan\delta_3$	12.684474	-2.448343	-1.302887	-0.908131

Convergence of the phases



The positive energy wave function



Last example: *pp* scattering using free waves

Let us take de following interaction:

$$V(r) = V_{short} + \frac{e^2}{r}$$

We now that for positive energies the wave function

$$\Psi(r \to \infty) \longrightarrow AF_c + BG_c$$

wirh F_c, G_c Coulomb functions. Let us define the following screened potential

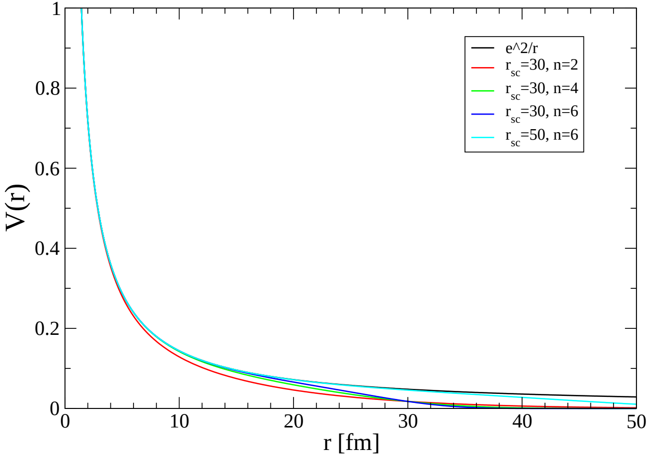
$$V_{sc}(r) = V_{short} + [e^{-(r/r_{sc})^n}]\frac{e^2}{r}$$

which, for specific values of r_{sc} and n tends to the original potential. Conversely, solving with the screened potential, the wave function behaves

$$\Psi_{n,r_{sc}}(r \to \infty) \longrightarrow AF + BG$$

with now F, G Bessel functions

The screened potential



pp scattering using free waves

The screened potential $V_{sc}(r < r_{sc}) = V(r)$ and therefore, the wave function $\Psi_{n,r_s c}$ verifies

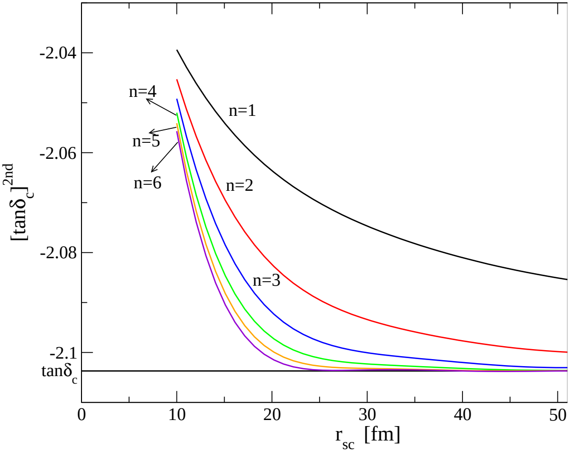
$$(T + V - E)\Psi_{n,r_{sc}} = 0$$

inside the interaction region $(r < r_{sc})$. And we can applied the integral relations:

i) $\Psi_{n,r_{sc}}$ is obtained using the screened potential:
$(T + V_{sc} - E)\Psi_{n,r_{sc}} = 0$
ii) The integral relations are used with the original V and the Coulomb functions

$$\begin{cases} B = -\frac{m}{\hbar^2} < \Psi_{n,r_{sc}}|T + V - E|F_c > \\ \\ A = \frac{m}{\hbar^2} < \Psi_{n,r_{sc}}|T + V - E|G_c > \end{cases}$$

$$[\tan \delta_c]^{2nd} = \frac{B}{A}$$



-2.04
-2.06
-2.08
-2.1
tanδ_c
[tanδ_c]^2nd
n=1
n=2
n=3
n=4
n=5
n=6
0
10
20
30
40
50
r_sc [fm]

Solving the Schrödinger equation

Exercise 1: *s*-wave solutions

In the following we will use the central, two-parameter potential:

$$V(r) = \begin{cases} -V_0 & r \leq r_0 \\ 0 & r > r_0 \end{cases}$$

The Schrödinger equation is

$$(H - E)\Psi = 0$$

For *s*-waves we use

$$\Psi = \frac{u(r)}{r} Y_{00}(\hat{r})$$

and the Schrödinger equation results

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

Solving the Schrödinger equation

A) Bound state solutions: $E < 0$

The Schrödinger equation

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

is now

$$\left(\frac{\partial^2}{\partial r^2} - \frac{mV(r)}{\hbar^2} - \kappa^2\right) u(r) = 0$$

To be solved after applying the boundary conditions:

$$\begin{cases} u(0) = 0 \\ u(r) = Be^{-\kappa r} \quad r > r_N \end{cases}$$

In addition the normalization condition

$$\int_0^\infty u^2(r)\, dr = 1$$

We proceed in the case of the two-parameter potential

$$V(r) = \begin{cases} -V_0 & r \leq r_0 \\ 0 & r > r_0 \end{cases}$$

The range of the force is $r_N = r_0$, and we distinguish two regions:

$$r < r_0 \rightarrow \left(\frac{\partial^2}{\partial r^2} + \frac{mV_0}{\hbar^2} - \kappa^2 \right) u(r) = 0$$

then $u(r) = A \sin k_0 r$

with $k_0^2 = \frac{mV_0}{\hbar^2} - \kappa^2$. And

$$r > r_0 \rightarrow \left(\frac{\partial^2}{\partial r^2} - \kappa^2 \right) u(r) = 0$$

with $u(r) = Be^{-\kappa r}$.

Matching conditions

The wave function Ψ and its derivative have to be continous. Therefore they have to be matched at $r = r_0$. These conditions can be applyied to the reduced wave function.

$$\begin{cases} A \sin k_0 r_0 = B\, e^{-\kappa r_0} \\ A k_0 \cos k_0 r_0 = -B \kappa e^{-\kappa r_0} \end{cases}$$

The first equation gives a relation between the two constants A and B. The ratio of the two equations can be used to find the condition for κ:

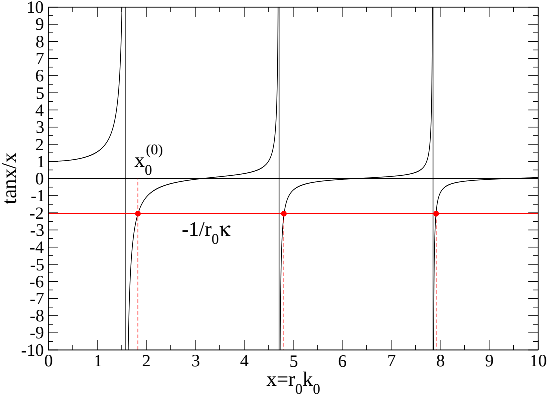
$$\frac{\tan k_0 r_0}{r_0 k_0} = -\frac{1}{r_0 \kappa}$$

calling $x = r_0 k_0$ the trascendental equation is

$$\frac{\tan x}{x} = -\frac{1}{r_0 \kappa}$$

It can be solved numerically, graphically, etc.

Graphical solution



Looking to the first sector $[x_0^{(0)}]^2 = r_0^2 m V_0/\hbar^2 - r_0^2\kappa^2$

or

$$\frac{\hbar^2}{m}\kappa^2 = E_d = V_0 - \frac{\hbar^2}{m r_0^2}[x_0^{(0)}]^2$$

This equation gives a relation between the binding energy E_d and the two parameters of the potential, V_0 and r_0. In order to fix completely the potential other observable has to be consider.

Let us return to the wave function:
$u(r) = Be^{-\kappa r_0} \sin k_0 r / \sin k_0 r_0$ for $r < r_0$
$u(r) = Be^{-\kappa r}$ for $r > r_0$.
The constant B is determined from normalization

$$e^{-2\kappa r_0} \int_0^{r_0} \frac{\sin^2 k_0 r}{\sin^2 k_0 r_0} dr + \int_{r_0}^{\infty} e^{-2\kappa r} dr = B^{-2}$$

$B \equiv A_s$ is the normalization constant. For the deuteron its value is $A_s = 0.878\,\mathrm{fm}^{-1/2}$

Solving the Schrödinger equation

B) Zero-energy solution: $E = 0$
The Schrödinger equation

$$\left(-\frac{\hbar^2}{m}\frac{\partial^2}{\partial r^2} + V(r)\right) u(r) = 0$$

is

$$r < r_0 \quad \left(\frac{\partial^2}{\partial r^2} + \frac{mV_0}{\hbar^2}\right) u(r) = 0 \qquad r > r_0 \quad \frac{\partial^2 u(r)}{\partial r^2} = 0$$

To be solved by applying the proper boundary conditions:

$$\begin{cases} u(0) = 0 \rightarrow u(r) = A \sin k_0 r & r < r_0 \\ \\ u(r) = r - a_S & r > r_0 \end{cases}$$

With a_S the scattering length and $k_0^2 = mV_0/\hbar^2$. The normalization condition is implicit in the coefficient equal to 1 of the regular solution.

Matching conditions

As before the reduced wave function and its derivative have to be matched at $r = r_0$.

$$\begin{cases} A \sin k_0 r_0 = r_0 - a_S \\ A k_0 \cos k_0 r_0 = 1 \end{cases}$$

From where the scattering length can be obtained

$$a_S = r_0 \left[1 - \frac{\tan k_0 r_0}{k_0 r_0} \right]$$

The wave function is $u(r) = \sin k_0 r / [k_0 \cos k_0 r_0]$ for $r < r_0$ and the effective range r_{eff} is

$$r_{\text{eff}} = \frac{2}{a_S^2} \int_0^{r_0} [u^2(r) - (r - a_S)^2] dr = r_0 \left[1 - \frac{r_0^2}{3a_S^2} - \frac{1}{k_0^2 a_S r_0} \right]$$

Close to threshold

For specific values of V_0 and r_0 the scattering length $a_S \to \pm\infty$. This happens when $k_0 r_0 = \sqrt{r_0^2 m V_0/\hbar^2} \to \pi/2$. In this region the bound or virtual state energy $E_d, E_v \to 0$. In fact, for bound state

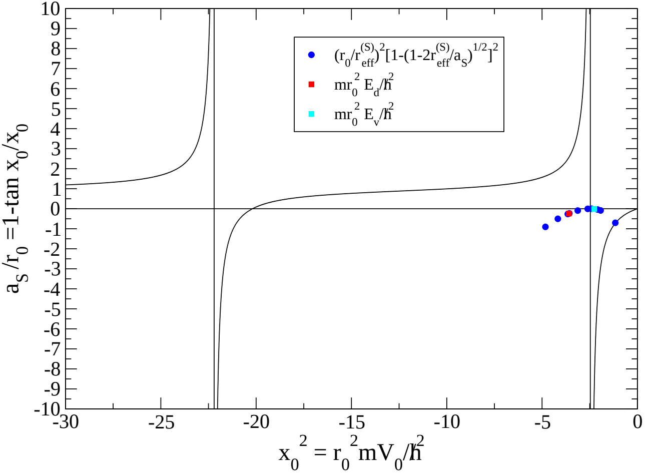
$$\frac{\tan x}{x} = -\frac{1}{r_0 \kappa}$$

with $x = r_0 k_0$ and $k_0^2 = \frac{mV_0}{\hbar^2} - \kappa^2$. Therefore when $\kappa \to 0$ the same condition results for $\frac{mV_0}{\hbar^2}$.

Moreover close to threshold we have demonstrated that

$$\kappa = \frac{1}{a_S} + \frac{r_{\text{eff}}}{2} \frac{1}{\kappa^2}$$

Close to threshold



Results

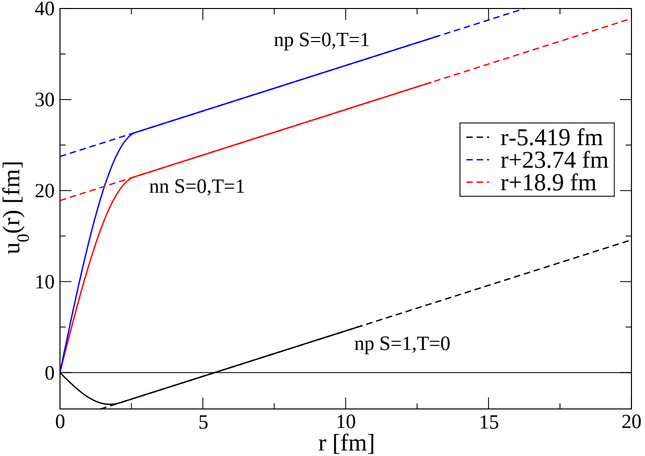
Some numerical results for the spin $S = 1$, $T = 0$ channel

V_0 MeV	r_0 fm	E_d MeV	a_1 fm	$r_{eff}^{(1)}$ fm	A_S $fm^{-1/2}$
-30.58	2.23	2.225	5.479	1.859	0.892
-33.73	2.10	2.224	5.410	1.767	0.877
-33.47	2.11	2.224	5.416	1.774	0.878
Exp.		2.224	5.419(7)	1.753(8)	0.878(1)

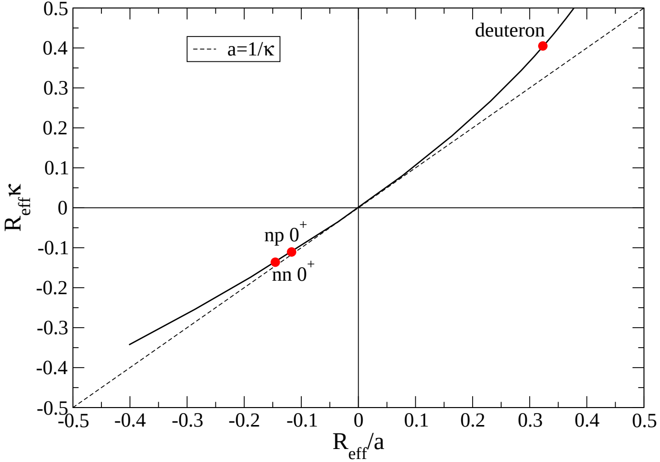
Some numerical results for the spin $S = 0$, $T = 1$ channel

np				*nn*			
V_0 MeV	r_0 fm	a_0 fm	$r_{eff}^{(0)}$ fm	V_0 MeV	r_0 fm	a_0 fm	$r_{eff}^{(0)}$ fm
-13.90	2.60	-23.74	2.72	-13.29	2.63	-18.90	2.78
-13.36	2.65	-23.74	2.77	-13.62	2.60	-18.90	2.75
Exp.		-23.74(2)	2.77(5)			-18.90(2)	2.75(1)

Zero-energy wave function



Universal concepts



Solving the Schrödinger equation

C) positive-energy solutions: $E > 0$
The Schrödinger equation

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

is in this case

$$r < r_0 \quad \left(\frac{\partial^2}{\partial r^2} + \frac{mV_0}{\hbar^2} + k^2\right) u(r) = 0 \qquad r > r_0 \quad \left(\frac{\partial^2}{\partial r^2} + k^2\right) u(r) = 0$$

To be solved by applying the proper boundary conditions:

$$\begin{cases} u(0) = 0 \rightarrow u(r) = A \sin q_0 r & r > r_0 \\ u(r) = \sin kr + \tan \delta_S \cos kr & r > r_0 \end{cases}$$

With δ_S the phase-shift and $q_0^2 = mV_0/\hbar^2 + k^2$.

Matching conditions

As before the reduced wave function and its derivative have to be matched at $r = r_0$.

$$\begin{cases} A \sin q_0 r_0 = \sin kr_0 + \tan \delta_S \cos kr_0 \\ A q_0 \cos q_0 r_0 = k \cos kr_0 - \tan \delta_S k \sin kr_0 \end{cases}$$

Fixing the energy E of the scattering process and using the potential parameters V_0, r_0 determined from the zero-energy and bound solutions, the following 2×2 system of equations is formed

$$\begin{cases} A \sin q_0 r_0 - \tan \delta_S \cos kr_0 = \sin kr_0 \\ A q_0 \cos q_0 r_0 + \tan \delta_S k \sin kr_0 = k \cos kr_0 \end{cases}$$

With $\hbar^2 k^2 / m = E$ and $q_0^2 = m V_0 / \hbar^2 + k^2$.

Effective function $S_k = k \cot \delta_S$

At low energies $k \cot \delta_S = -\frac{1}{a_S} + \frac{r_{eff}^{(S)}}{2} k^2 + \dots$