TALENT Course 6: Theory for exploring nuclear reaction experiments
Exercises 1: Monday Week 1
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Analytical/Mathematical exercises

1. **Scattering boundary conditions**:

   The scattering phase shift, for an orbital angular momentum ℓ between a projectile and a target nucleus, $\delta_\ell \equiv \delta_\ell(E_{cm})$, is a function of the collision energy in their centre-of-mass E_{cm}. Its effects can also be be summarised in terms of the partial wave transition matrix or S-matrix elements, defined as

   $$T_\ell = \exp(i\delta_\ell)\sin\delta_\ell\ , \qquad S_\ell = \exp(2i\delta_\ell)$$

   The asymptotic forms of the scattering wave functions, i.e. for $E_{cm} > 0$, outside of the range of the nuclear potentials, are expressed in terms of the known regular (sine-like) and irregular (cosine-like) solutions of the radial Schrödinger equation, $F_\ell(k,r)$ and $G_\ell(k,r)$ and their outgoing-waves (H_ℓ^+) and ingoing-waves (H_ℓ^-) combinations

   $$H_\ell^\pm(k,r) = G_\ell(k,r) \pm iF_\ell(k,r)\ .$$

   Show that the following three alternative asymptotic forms for the scattering wave function are equivalent:

   $$\begin{aligned} u_\ell(k,r) &= e^{i\delta_\ell}\left[\cos\delta_\ell F_\ell(k,r) + \sin\delta_\ell G_\ell(k,r)\right] \\ &= \Big[F_\ell(k,r) + T_\ell H_\ell^+(k,r)\Big] \\ &= \frac{i}{2}\Big[H_\ell^-(k,r) - S_\ell H_\ell^+(k,r)\Big]\ . \end{aligned}$$

2. **Resonance descriptions**:

   For projectile-target scattering at centre-of-mass energies E_{cm} near to a single, isolated and narrow (Γ small) resonance (of angular momentum ℓ at energy E_r) in the colliding system, the phase shift is often written:

   $$\delta_\ell(E_{cm}) = \arctan\left(\frac{\Gamma/2}{E_r - E_{cm}}\right)\ \ (\text{modulo } \pi)\ .$$

   Note that as as E_{cm} is increased from below to above E_r then δ_ℓ increases, passing through $\pi/2$ (modulo π).

   The contribution to the total elastic scattering cross section from this partial wave for energies near the resonance, $E_{cm} \approx E_r$, is

   $$\sigma_\ell(E_{cm}) = \frac{4\pi}{k^2}(2\ell+1)|T_\ell(E_{cm})|^2$$

where T_ℓ is the partial wave transition matrix element of Question 1. Show that the cross section exhibits a *Briet-Wigner*–like resonance peak

$$\sigma_\ell(E_{cm}) = \frac{4\pi}{k^2}(2\ell+1)\frac{(\Gamma/2)^2}{(E_{cm}-E_r)^2+(\Gamma/2)^2} \ .$$

Show also that corresponding partial wave S-matrix element has the form

$$S_\ell(E_{cm}) = \frac{E_{cm}-E_r-i\Gamma/2}{E_{cm}-E_r+i\Gamma/2}$$

and hence has a mathematical pole at the complex energy $E_r - i\Gamma/2$.

3. **Continuum bins definitions**:
Plane wave (momentum) eigenstates in three dimensions, $\langle \mathbf{r}|\mathbf{k}\rangle = \exp(i\mathbf{k}\cdot\mathbf{r})$, have normalisation

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \int d\mathbf{r}\ \exp(-i\mathbf{k}\cdot\mathbf{r})\exp(i\mathbf{k}'\cdot\mathbf{r}) = (2\pi)^3\delta(\mathbf{k}-\mathbf{k}') \ .$$

Scattering states $\phi^{(+)}_{\mathbf{k}}(\mathbf{r})$ can be shown to share the same normalisation condition, that is

$$\langle \phi^{(+)}_{\mathbf{k}}|\phi^{(+)}_{\mathbf{k}'}\rangle = (2\pi)^3\delta(\mathbf{k}-\mathbf{k}') \ .$$

It can be shown, using the partial wave expansions of these scattering wave functions, that the *radial* parts of these wave functions $u_\ell(k,r)$ satisfy the condition

$$\int_0^\infty dr\ u^*_\ell(k,r)u_\ell(k',r) = \frac{\pi}{2}\delta(k-k') \ .$$

Assuming this property of the radial wave functions, show that *continuum bin* wave functions $\hat{u}_i(r)$ constructed as linear superpositions of these radial wave functions over different, non overlapping, ranges of momenta Δk_i (or energies) with some optional weight function $g(k)$,

$$\hat{u}_i(r) = C_i\int_{\Delta k_i} dk\, g(k)u_\ell(k,r) \ , \ \ \Delta k_i = k_i - k_{i-1}$$

are orthogonal. That is,

$$\int_0^\infty dr\ \hat{u}^*_i(r)\hat{u}_j(r) = 0 \ \ \text{if} \ \ i\neq j \ .$$

Find also the correct choices of the constants C_i so that the $\hat{u}_i(r)$ are orthonormal, that is they behave like bound state wave functions:

$$\int_0^\infty dr\ \hat{u}^*_i(r)\hat{u}_j(r) = \delta_{ij} \ .$$

This means that excitations to and between different bin states can be treated using the same mathematical and numerical techniques as were developed for inelastic excitations of bound excited states.

4. **Continuum bins example**: Using the results of the previous question, or otherwise, show that, for s-wave scattering states $u_0(k, r)$, if these are replaced by plane wave states, i.e.

$$u_0(k, r) = \sin kr$$

then the corresponding bin states, for $g(k) = 1$, are

$$\hat{u}_i(r) = C_i \int_{k_{i-1}}^{k_i} dk\, u_0(k, r) = \sqrt{\frac{2}{\pi \Delta k_i}} \left[\frac{\cos k_{i-1} r}{r} - \frac{\cos k_i r}{r} \right].$$

The spreadsheet `bins.xls` on the Exercises web-page calculates the form of these $\hat{u}_i(r)$ for two pairs of values of k_i and k_{i-1} of your choosing, and also shows the calculated norms and the orthogonality integral for the $\hat{u}_i(r)$ for the two chosen bin ranges.

Introductory computational exercises

1. Find the separation energies and graph the radial wave functions of all the states of a neutron that are bound in a mass $A = 40$ nucleus. Assume that the real central Woods-Saxon binding potential is fixed and is $(V, r, a) =$ (30.0 MeV, 1.25 fm, 0.65 fm). You should first assume that $V_{so} = 0.0$ and then that $V_{so} = 6.0$ MeV. What are the differences? Use the program `bound`. Is this potential depth realistic for say ^{40}Ca?

2. Calculate and plot the phase shifts in the s, p, d and f-partial waves (ℓ =0, 1, 2 and 3) for a neutron scattering in the same real potential $(V, r, a) =$ (30.0 MeV, 1.25 fm, 0.65 fm) for $0 < E_{cm} < 8$ MeV. Interpret their behaviour in terms of the number of bound states present in each partial wave that were found in Question 1 above. Use the program `scatter` with no spin-orbit force.

3. Calculate and plot the phase shifts δ_ℓ and the partial wave elastic cross sections $\sigma_\ell(E_{cm})$ in the f-partial wave ($\ell = 3$) for this same problem, for $0 < E_{cm} < 8$ MeV, starting with the real potential $(V, r, a) =$ (30.0 MeV, 1.25 fm, 0.65 fm).

   Deduce the E_{cm} value at which $\delta_3 = 90$ degrees. Find and plot the corresponding positions E_{cm} at which $\delta_3 = 90$ degrees as a function of increasing V (i.e. as the well is made deeper). Eventually the f-wave neutron state will also become bound. Extend your plot to negative (bound) E_{cm} values versus V to include these bound state eigenvalues of the f-wave state. Use programs `scatter` and `bound`.

4. Run the programs `bound` and `scatter` for any system of two particles/nuclei of your choice (e.g. that in Question 1). Assume the particles interact with a fixed real potential. `scatter` does not include spin so assume the valence particle also has spin zero in `bound` also. Graph the bound and a scattering wave function for the same chosen ℓ value and show that these radial wave functions are orthogonal.

5. The separation energy of a neutron from ^{40}Ca to form the ground state of ^{39}Ca is (see e.g. http://ie.lbl.gov/toi2003/MassSearch.asp) 15.641 MeV and the ^{39}Ca ground state has spin and parity $3/2^+$.

   Assuming a potential geometry of $r = 1.25$ fm and $a = 0.7$ fm and a spin orbit force of 6.0 MeV, find the potential depths V needed to describe the least bound neutron and proton states in ^{40}Ca. Are they equal? Should they be? Calculate the eigenenergies of all of the bound neutron and proton eigenstates in these (now fixed depth) potential wells.

6. How well is the experimental splitting of the $1f_{7/2}$ and $1f_{5/2}$ states in ^{41}Ca reproduced when using the standard potential geometry (1.25, 0.65) and $V_{so} = 6$ MeV and when using radius parameters deduced from a Skx Skyrme interaction Hartree Fock calculation, i.e. use geometry (r_0, 0.70) and $V_{so} = 6$ MeV.

7. Find the real potential strengths that are needed in the $\ell = 0$ and $\ell = 2$ states of the deuteron + alpha-particle system to give a reasonable description of the low-lying (both bound and resonant) isospin T=0 states of ^{6}Li (you will need to use `bound` and `scat`). You should assume that the potential geometry has $R = 1.90$ fm (note R not r_0), $a = 0.65$ fm and that the spin orbit force is $V_{so} = 2.05$ MeV.

   (see e.g. http://www.tunl.duke.edu/nucldata/ourpubs/ourpubs.shtml)

   Use the program `scat_one` (which prints the radial wave function at a single scattering energy) to look at the deuteron + alpha-particle relative motion wave functions at the resonance positions of your potentials.

8. Calculate and plot the partial wave S-matrix elements S_ℓ, i.e. the real and imaginary parts and $|S_\ell|$ for neutron scattering from a mass 28 target in the following complex potentials with real part (V, r, a) = (50.0 MeV, 1.25 fm, 0.65 fm). Assume volume Woods-Saxon shaped absorptive (imaginary) terms with (W_v, r_v, a_v) = (10.0 MeV, 1.20 fm, 0.60 fm), (15.0 MeV, 1.20 fm, 0.60 fm) and (20.0 MeV, 1.20 fm, 0.60 fm) at E_{cm} = 10, 40 and 100 MeV, respectively.

   Compare the values of ℓ for which $|S_\ell| \approx 0.5$ with the values that might be expected based on the radii of the optical potentials and the neutron wave numbers k at these three energies.

9. Calculate and plot the Hartree-Fock densities for neutrons and protons in neutron-deficient ^{31}Ar and neutron-rich ^{25}Ne. Use the program `dens` and the SkX Skyrme interaction.