TALENT Course 6: Theory for exploring nuclear reaction experiments
Supplementary handout 1: Monday Week 1
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Two-particle bound and scattering states calculations

Introduction

Codes provided that solve the (non-relativistic) radial Schrödinger equation

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2}[E_{cm} - V(r)]\right) u_\ell(r) = 0 \quad , \tag{1}$$

for bound ($E_{cm} < 0$) and scattering ($E_{cm} > 0$) solutions for a system of two particles of masses A_1 (projectile) and A_2 (target), and reduced mass μ, interacting via a potential $V(r)$, are `bound` and `scatter`. The potential $V(r)$ will, in general, consist of short ranged interactions $V_N(r)$ plus the Coulomb interaction $V_C(r)$ when the projectile (Z_1) and target (Z_2) are charged. For bound states $V_N(r)$ is simply assumed to be a real central interaction with a Woods-Saxon shape. For scattering states $V_N(r)$ will in general be assumed to be an arbitrary complex central interaction based on the usual volume and surface Woods-Saxon shapes, as follows

$$V(r) = V_N(r) + V_C(r) = \left\{ -\frac{V_0}{(1+e^{X_0})} - i\frac{W_v}{(1+e^{X_v})} - i\frac{4W_s e^{X_s}}{(1+e^{X_s})^2} \right\} + V_C(r). \tag{2}$$

So, for an attractive (negative) real potential and an absorptive (negative) imaginary potential the strengths V_0, W_v and W_s are each defined to be positive. In the above equation the factors X_i are

$$X_i = (r - R_i)/a_i \ , \qquad R_i = r_i A_2^{1/3} \ , \tag{3}$$

with r_i and a_i the usual radius and diffuseness parameters (typically of order 1.2 and 0.6 fm, respectively). The Coulomb interaction $V_C(r)$ for charged particles is assumed to be that of a uniformly charged sphere with a radius R_C, taken here to be equal to that assigned to the real central interaction $R_C = R_0 = r_0 A_2^{1/3}$, and is then

$$V_C(r) = \frac{Z_1 Z_2 e^2}{r}, \qquad r > R_C \tag{4}$$

$$= \frac{Z_1 Z_2 e^2}{2R_C}\left[3 - \left(\frac{r}{R_c}\right)^2\right]. \qquad r \le R_C. \tag{5}$$

Spin-orbit interactions are not necessary for the currently required outcomes and the strengths can be set to zero if programs prompt for them for the time being.

Outputs from `scatter` are the radial wave functions $u_\ell(r)$ (see Eq. 14), the phase shifts δ_ℓ and the partial wave T- and S-matrices, $T_\ell(E_{cm}) = e^{i\delta_\ell}\sin\delta_\ell$ and $S_\ell(E_{cm}) = e^{2i\delta_\ell}$. The integrated elastic scattering cross section is

$$\sigma(E_{cm}) = \sum_{\ell=0}^{\infty} \sigma_\ell(E_{cm}) = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)|T_\ell(E_{cm})|^2 \ . \tag{6}$$

The contributions from each partial wave ℓ, are

$$\sigma_\ell(E_{cm}) = \frac{4\pi}{k^2}(2\ell+1)|T_\ell(E_{cm})|^2 \tag{7}$$

and are also output. For real $V_N(r)$, δ_ℓ is also real and then $|T_\ell(E_{cm})|^2 = \sin^2\delta_\ell$.

Program bound

This program works in terms of the positive *separation energy* S_{cm} of the bound particles rather than the negative energy eigenvalue E_{cm}, with $S_{cm} = -E_{cm}$. The program can find either

(a) the bound states in a specified fixed potential, or

(b) the potential that will produce a bound state with a particular separation energy.

The program is self documenting, asking for the required input parameters. If used without spin-orbit forces, respond in any way to the spin- and j-value requests and return zero for the spin-orbit potential strength. The real radial wave functions $u_\ell(r)$ for the bound states are defined such that

$$\int_0^\infty dr r^2 [u_\ell(r)/r]^2 = \int_0^\infty dr [u_\ell(r)]^2 = 1, \tag{8}$$

and thus behave as $r^{\ell+1}$ near the origin. The wave functions are written as $(r, u_\ell(r))$ pairs to the file `bound.xxx` for graphical use and as $u_\ell(r)/r$ values to the file `bd.xxx` for further computation and interface with other codes. The distinguishing trailer `xxx` is user-specified.

The wave functions are calculated for the range of radii $0 \le r \le 30$ fm.

The number of nodes in the radial wave function starts with $n = 0$ for the lowest energy state of a given ℓ, so the zeroes of the wave function at the origin and at infinity are not counted in the node count.

Program scatter

A specimen data set `scatter.one` contains the specification of the required inputs.

```
projectile:                    mass charge
target:                        mass charge
```

```
matching radius (fm)       (typically 15. fm)
integration step length    (typically 0.1 fm)
centre of mass energies:    e_min     e_max
number of energies:         nener
partial waves:              l_min   l_max
Real Woods-Saxon (volume)   V_0   r_0   a_0
Imag Woods-Saxon (volume)   W_v   r_v   a_v
Imag Woods-Saxon (surface)  W_s   r_s   a_s
```

The user-specified filename trailer of the data set (here `one`) will then label all output files from this data set, `phases.one`, etc. and can be used to identify output from different runs.

The suggested matching radius of 15.0 fm, beyond which $V_N(r)$ is assumed to vanish (see Appendix), and integration step of 0.1 fm should be adequate for all of the cases needed here.

The output files produced for a data set `scatter.xxx` are as follows. The phase shifts, etc. are ordered by the scattering energy for each value of ℓ, with an `xmgr` recognised separator.

```
phases.xxx    phase shifts in degrees (real V_N): Ecm delta
potent.xxx    the potential V_N(r): r  Re.V_N  Im.V_N  V_C
smatrix.xxx   partial wave S-matrix elements: ell Re.S Im.S |S|
tmatrix.xxx   partial wave T-matrix elements: ell Re.T Im.T
wavefun.xxx   radial wave functions: r  Re.u   Im.u
sigmas.xxx    partial cross sections of Eq.(7) Ecm  sigma (fm**2)
```

The routines `scatter` and `bound` are intended to provide a foundation from which to understand the behaviours of outputs from a set for potential scattering and bound states problems. The intention is to understand those aspects of scattering that guide intuition and that are needed as input to larger-scale reaction calculations. We can use these programs later to test approximate scattering theories by comparison with the exact results and also to examine and fine-tune input we put into reaction codes and so test individual inputs.

Appendix A: Outline of solution

(1) The codes calculate numerically the solutions of the radial differential equations in the presence of the potentials $V(r)$, for each relative orbital angular momentum (or partial wave) ℓ,

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2}[E_{cm} - V(r)]\right) u_\ell(r) = 0 \quad . \tag{9}$$

(2) The required (physical) solutions are regular (i.e. $u_\ell(r) = 0$) at the origin. Here, μ is the projectile-target reduced mass.

(3) Outside of the range of the nuclear (Woods Saxon) interactions, where $V(r) \to V_C(r)$, the radial equation can be written

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\eta k}{r} + k^2\right) u_\ell(r) = 0 \tag{10}$$

where η is the Sommerfeld (Coulomb) parameter and k is the wavenumber, $k^2 = 2\mu E_{cm}/\hbar^2$.

(4) The regular, $F_\ell(\eta, kr)$, and irregular, $G_\ell(\eta, kr)$, (Coulomb function) solutions of this equation are well known and standard functions.

To outline the solution, consider the scattering of uncharged particles, for which $\eta = 0$. Numerical integration is performed away from the origin using the Numerov algorithm (outlined in the following section) using an integration step length h (to be specified).

The numerical solution is then matched to the required physical solution at a radius R_{match} (to be specified), outside of the ranges R of the Woods Saxon potentials, i.e. for which $V(r) = V_N(r) = 0,\ r \geq R$. For these radii

$$\begin{aligned} u_\ell(r) &= A_\ell F_\ell(0, kr) + B_\ell G_\ell(0, kr) \quad , \quad (r > R) \quad , & (11) \\ &\to C_\ell \sin(kr - \ell\pi/2 + \delta_\ell) \quad , \quad (r \to \infty) \quad , & (12) \end{aligned}$$

where $F_\ell(0, kr)$ and $G_\ell(0, kr)$ are the solutions of Eq. 10 for $\eta = 0$ – the free particle (no potential) radial equation.

These have very simple forms for small ℓ,

$$\begin{aligned} F_0(0, kr) &= \sin(kr) \quad , & G_0(0, kr) &= \cos(kr) \quad , \\ F_1(0, kr) &= \frac{\sin(kr)}{kr} - \cos(kr) \quad , & G_1(0, kr) &= \frac{\cos(kr)}{kr} + \sin(kr) \quad , \end{aligned}$$

and for other ℓ satisfy the recurrence formula

$$F_{\ell+1}(0, kr) = \frac{2\ell+1}{kr} F_\ell(0, kr) - F_{\ell-1}(0, kr) \quad ,$$

and similarly for the G_ℓ. They have the asymptotic forms

$$\begin{aligned} F_\ell(0, kr) &\to \sin(kr - \ell\pi/2) \quad , \\ G_\ell(0, kr) &\to \cos(kr - \ell\pi/2) \quad . \end{aligned}$$

The matching to the physical solution at radii $r > R$ is carried out at two radii r_1 and r_2. That is the simultaneous equations

$$\begin{aligned} u_\ell(r_1) &= A_\ell F_\ell(0, kr_1) + B_\ell G_\ell(0, kr_1) \quad , \\ u_\ell(r_2) &= A_\ell F_\ell(0, kr_2) + B_\ell G_\ell(0, kr_2) \quad , \end{aligned}$$

are solved for A_ℓ, B_ℓ.

These constants of solution A_ℓ and B_ℓ determine the scattering phase shift, according to $A_\ell = C_\ell \cos\delta_\ell$, $B_\ell = C_\ell \sin\delta_\ell$, with $C_\ell = \sqrt{A_\ell^2 + B_\ell^2}$, and hence $\delta_\ell = \arctan(B_\ell/A_\ell)$.

The partial wave T- and S-matrix elements $T_\ell(E_{cm})$ and $S_\ell(E_{cm})$ are

$$T_\ell(E_{cm}) = e^{i\delta_\ell} \sin\delta_\ell, \qquad S_\ell(E_{cm}) = e^{2i\delta_\ell}. \tag{13}$$

The radial wave function defined by Eq. 12 is useful as it real for the case that $V(r)$ is real. The wave function printed from `scatter.f` is defined such that

$$u_\ell(r) \to \cos\delta_\ell F_\ell(\eta, kr) + \sin\delta_\ell G_\ell(\eta, kr) \quad , \quad (r > R) \ . \tag{14}$$

Appendix B: Numerical outline

The Numerov algorithm for the solution of a homogeneous second order ordinary differential equation of the general form

$$u''(r) = \mathcal{K}(r) u(r) \quad ,$$

using a constant step/interval h, is based on the relationship

$$\left[1 - \frac{h^2}{12}\mathcal{K}(r+h)\right] u(r+h) = \left[2 + \frac{5h^2}{6}\mathcal{K}(r)\right] u(r) - \left[1 - \frac{h^2}{12}\mathcal{K}(r-h)\right] u(r-h) \quad .$$

The error involved is of order h^6 and is thus rather accurate for reasonably small h. In the context of the radial Schrödinger equation we must associate

$$\mathcal{K}(r) \equiv \mathcal{K}_\ell(r) = \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2}[V(r) - E_{cm}] \quad .$$

The solution is computed iteratively, from a knowledge of the behaviour of the regular solution at $r = 0$ and $r = h$, $\propto (kr)^{\ell+1}$. Inspection will show that some care needed in specifying these starting conditions for the case that $\ell = 1$. This special case is taken care of in the program `scatter.f`.

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