Problem Set 11
Physics 480 / Fall 1999
Professor Klaus Schulten

Problem 1: Scattering by a Spherical Potential Well

Consider the scattering of electrons by a spherically symmetric potential well described by a potential

$$U(r) = \begin{cases} U_o\,, & \text{for} \quad r < a \\ 0\,, & \text{for} \quad r > a \end{cases} \tag{1}$$

where $a = 1$Å. Assume a kinetic energy of the incoming electron beam of $E = 1$ KeV. The well depth is $U_o = -100$ eV. Employ `Mathematica` tools where necessary. Describe the scattering through a partial wave expansion, i.e., assume for the wave function

$$\psi(\vec{r}) = \sum_{\ell=0}^{\infty} v_\ell(k,\, r)\, P_\ell(\cos\theta) \tag{2}$$

where k is defined through $\hbar^2 k^2/2m_e = E$. We derived in class that for potentials which vanish rapidly enough for large r the radial wave functions behave asymptotically ($r \to \infty$) as

$$v_\ell(k,\, r) \sim \frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)}{kr}\,. \tag{3}$$

The corresponding differential cross section is

$$\frac{d\sigma}{d\Omega} = \left| \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\delta_\ell} \sin\delta_\ell\, P_\ell(\cos\theta) \right|^2 . \tag{4}$$

(a) Show that the total cross section defined through

$$\sigma_{tot} = 2\pi \int_0^\pi \sin\theta\, d\theta \frac{d\sigma}{d\Omega} \tag{5}$$

is given by

$$\sigma_{tot} = \sum_{\ell=0}^{\infty} \sigma_\ell \tag{6}$$

where

$$\sigma_\ell = \frac{4\pi}{k^2}\,(2\ell+1)\sin^2\delta_\ell\,. \tag{7}$$

(b) Argue why in (4, 6) only ℓ values up to about $\ell_{max} = k\,a$ contribute. How large is ℓ_{max}.

(c) Argue why the radial wave functions for the present scattering problem are given by

$$v_\ell(k,\, r) \;=\; \begin{cases} \alpha_\ell\, j_\ell(Kr)\,, & \text{for} \quad r\,<\,a \\ \beta_\ell\, j_\ell(kr)\,+\,\gamma_\ell\, n_\ell(kr)\,, & \text{for} \quad r\,>\,a \end{cases} \tag{8}$$

where j_ℓ, n_ℓ denote the spherical Bessel functions introduced in class and where K is defined through $\hbar^2 K^2/2m_e \;=\; E\;-\;U_o$. (Note: the spherical Bessel functions $j_\ell(z)$, $n_\ell(z)$ are related to the regular and irregular Bessel functions $J_m(z)$ and $N_m(z)$, respectively, as follows

$$j_\ell(z) \;=\; \sqrt{\frac{\pi}{2z}}\, J_{\ell+\frac{1}{2}}(z)\,, \quad n_\ell(z) \;=\; \sqrt{\frac{\pi}{2z}}\, N_{\ell+\frac{1}{2}}(z)\,. \tag{9}$$

The functions $J_m(z)$ and $N_m(z)$ correspond to the `Mathematica` functions **BesselJ[m,z]** and **BesselY[m,z]**.

(d) Determine the constants β_ℓ and γ_ℓ in (8) and from the result evaluate the scattering phase shifts δ_ℓ as defined in (3). Plot δ_ℓ as a function of ℓ.

(e) Plot the differential cross section as a function of θ.

(f) State the value of the total cross section.

Problem 2: Resonant Scattering States for a Spherical Potential Well

A resonant scattering state is defined by a sharp maximum of the corresponding (total) scattering cross section σ_{tot} as a function of the energy $E = \hbar^2 k^2/2m$ of the scattered particle. The purpose of this problem is to investigate the resonant states for scattering by a spherical potential well of radius a and depth U_o. It is convenient to chose length and energy units given by a, and $4 \times U_o^{(\min)}$, where $U_o^{(\min)}$ represents the minimum value of U_o for which the well can accommodate a bound state.

(a) Show that

$$U_o^{(\min)} \;=\; \frac{\pi^2 \hbar^2}{8ma^2} \tag{10}$$

What is the minimum value of U_o for the well to accommodate two bound states of zero angular momentum?

(b) By employing the new length and energy units, write down the expression of the scattering cross section $\sigma_{tot}(k, U_o)$ as a sum of partial wave contributions $\sigma_\ell(k, U_o)$ as defined in (6, 7).

(c) For $\ell = 0, 1, 2$ and 3 calculate numerically (e.g., by employing `Mathematica`) $\sigma_\ell(k, U_o)$, and present the results of your calculations as a density plot (e.g., by using the `Mathematica` **DensityPlot** command) of σ_ℓ *vs.* k $(0 < k < 3)$ and $\sqrt{U_o}$ $(0 < \sqrt{U_o} < 2.5)$.

(d) Calculate numerically σ_{tot} for the same values of k and $\sqrt{U_o}$ as in (c), and present your result as a density plot. For practical purposes, you can cut off the infinite sum over the angular momentum at $\ell_{\max} = 4k$. Your plot should look similar to the one given in Fig. 1.

(e) Identify the values of k and $\sqrt{U_o}$ ("resonance island") for which resonant scattering occurs, *i.e.*, for which in the figure obtained in (d) the largest values for σ_{tot} arise. Then, by comparing this plot, with the ones obtained in(c), identify for each "resonance island" the ℓ component of the partial wave expansion that actually exhibits the resonance.

(f) Calculate numerically and plot the radial wave functions corresponding to the first three (lowest in energy) resonant states identified in (e).

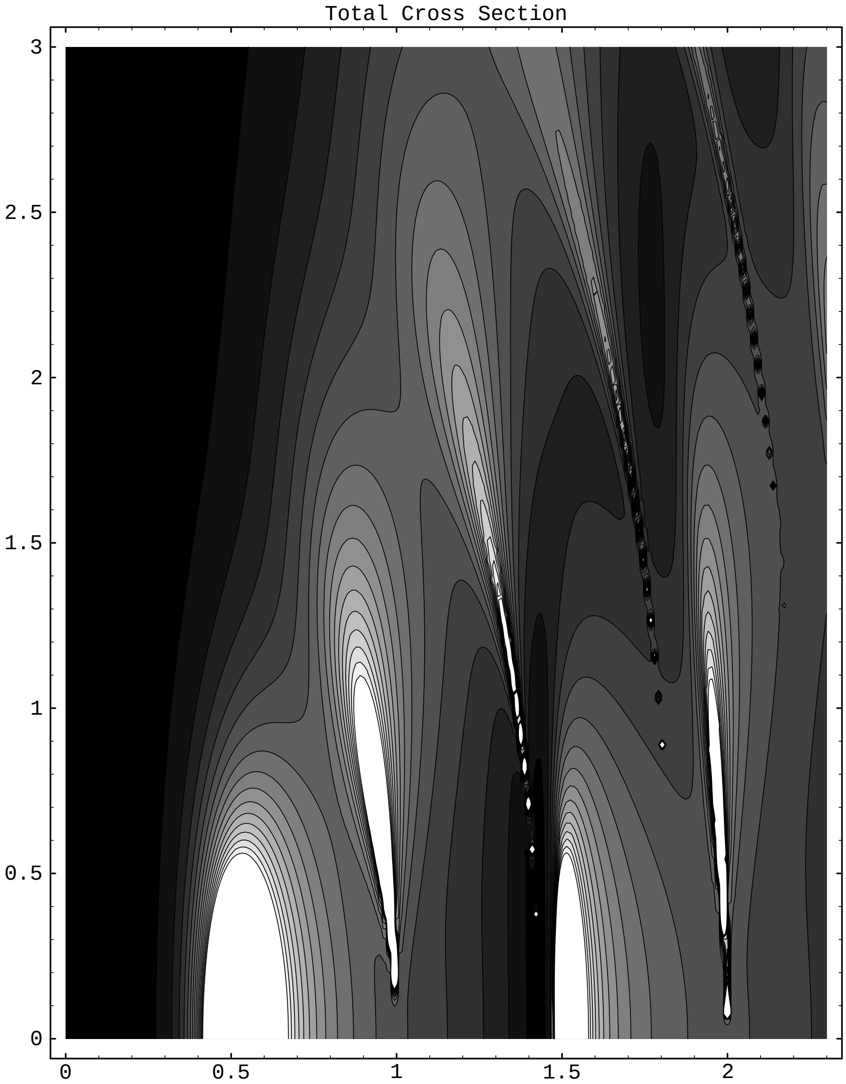

Figure 1: Density plot of the total cross section σ_{tot}, for a square well potential, as a function of $\sqrt{U_o}$ (horizontal axis) and k (vertical axis).

The problem set needs to be handed in by Thursday, December 9. The web page of Physics 480 is at `http://www.ks.uiuc.edu/Services/Class/PHYS480/`