5 Quantum Mechanics

5.2 Electron Scattering (7 units)

This project relies on knowledge of material from the course Applications of Quantum Mechanics*.*

1 Introduction

Scattering theory can be used to compute what happens when a beam of electrons is fired towards a target object. The electrons collide with the object and are scattered off in new directions. The angular distribution of the outgoing electrons is described by a sum of contributions, in which the simplest term corresponds to an isotropic distribution. If the energy of the incoming electron is not too large, this isotropic contribution dominates the distribution. This situation is called s-wave scattering.

2 Theory

The electrons are incident on a target that is located at the origin and is decribed by an isotropic interaction potential $U(r)$. The time-independent Schrodinger equation for the outgoing electrons has a general solution

$$\psi(r,\theta) = \sum_{l=0}^{\infty} \frac{\chi_\ell(r)}{r} P_\ell(\cos\theta) \tag{1}$$

where ψ is the wave-function, P_ℓ is the Legendre Polynomial of order ℓ, and χ_ℓ satisfies

$$\frac{d^2\chi_\ell}{dr^2} + \left[k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\right]\chi_\ell = 0 \tag{2}$$

with boundary condition $\chi_\ell(0) = 0$. The constant k is determined by the energy E of the incoming electrons, with E proportional to k^2.

Suppose that the target has radius r_0 and that $U(r) = 0$ for $r > r_0$. Then for large r one has asymptotically $\chi_\ell(r) \approx A_\ell \sin(kr - \frac{1}{2}l\pi + \delta_\ell)$, where δ_ℓ is the (k-dependent) phase shift of the ℓ^{th} partial wave. The total scattering cross-section σ is given by

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell \,. \tag{3}$$

The s-wave contribution to (1) is the term with $\ell = 0$. The associated (k-dependent) cross section is therefore $\sigma_0 = (4\pi/k^2)\sin^2\delta_0$. To characterise the low-energy behaviour, a useful quantity is the scattering length a, which is defined by $(1/a) = \lim_{k\to 0}[-k\cot\delta_0(k)]$.

For further information on this theory, see for example

1. L.I. Schiff, *Quantum Mechanics*, §19. Scattering by spherically symmetric potentials.

2. S. Gasiorowicz, *Quantum Physics*, Ch. 24. Collision theory.

3 Computation

You will write a program to investigate numerically the relation between the phase shift δ_0 and k. We consider the potential

$$U(r) = \begin{cases} -U_0\left(1-\frac{r}{\pi}\right)^3 & r \leqslant \pi \\ 0 & r > \pi \end{cases} . \tag{4}$$

Programming Task: Numerically solve (2) for $\chi_0(r)$ (i.e. the case $\ell = 0$) taking $\chi_0(0) = 0$ and $\chi_0'(0)$ an arbitrary value. (You should verify that this arbitrary value only affects the normalisation of the wavefunction.)

Question 1 Explain your choice of numerical method and discuss the accuracy of the solutions you obtain.

Question 2 Investigate the solutions for χ_0 as you vary k in the range 0 to 5 and U_0 from 0 to 10. Discuss the dependence of the wavefunction on U_0 for a few different values of k. Your report should include a few plots to support your observations, which should include the case $U_0 = 0$.

Note: throughout this project, you should provide graphs that illustrate clearly the similarities and differences between the various cases. Large numbers of graphs are *very unlikely to be effective* in communicating this information.

Programming Task: Modify your program to calculate δ_0, using the formula

$$\tan\delta_0 = \frac{\chi_0(r_2)\sin kr_1 - \chi_0(r_1)\sin kr_2}{\chi_0(r_1)\cos kr_2 - \chi_0(r_2)\cos kr_1} \tag{5}$$

where r_1 and r_2 are two r-values in $r > \pi$. (This formula can be derived from the asymptotic expression for χ_ℓ given in the Theory section.) It is conventional that δ_0 depends continuously on k and that $\delta_0 \to 0$ as $k \to \infty$, you should explain how you ensured that your results are consistent with this convention.

Question 3 Explain how a poor choice of r_1 and r_2 in Equation (5) can lead to a large error in δ_0. How did you avoid this? Note also that Equation (5) has multiple solutions for δ_0: explain which solution you have taken.

Question 4 For a few values of U_0, compute the phase shift and the cross-section as functions of k, with $0 < k < 5$. Plot graphs of these quantities. Take care to resolve the behaviour near $k = 0$.

Question 5 For the results of Question 4, plot the phase shift δ_0 as a function of U_0, for some small value(s) of k. Give a physical (quantum-mechanical) interpretation of the observed behaviour.

Question 6 Still for the results of Question 4, plot the cross section σ as a function of U_0 (always for small k). How are the features of this curve (extrema, etc) related to physical properties of the the scatterer?

Question 7 Using again the results of Question 6, determine (numerically) the scattering length a from the small-k behaviour of δ_0. Is the result consistent with your results for the cross section σ in question 5?

