PHY 304, II-Semester 2023/24, Assignment 5 solution

(1) Optical theorem: [10 pts] Use the partial wave expansion of the scattering amplitude $f(\theta)$ to show that the total scattering cross section σ is given by

$$\sigma = \frac{4\pi}{k}\mathrm{Im}[f(0)], \tag{1}$$

where k is the scattering wavenumber and $f(0)$ the forward scattering amplitude. This is known as the "optical theorem".

Solution:

We can write the scattering amplitude from Eq. (8.19) in lecture notes as,

$$f(\theta) = \sum_{l=0}^{\infty}(2l+1)a_l p_l(cos\theta). \tag{2}$$

Inserting the value of $a_l = \frac{1}{k}e^{i\delta_l}sin\delta_l$ *from Eq. (8.30) of lecture notes into* (2) *we get the differential scattering cross-section as,*

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{k^2}\left|\sum_{l=0}^{\infty}(2l+1)\exp(i\delta_l)P_l(\cos\theta)\sin\delta_l\right|^2 \tag{3}$$

We know that the total scattering cross-section is,

$$\begin{aligned}\sigma &= \int \sigma(\theta)d\Omega \\ &= \int_0^{2\pi}\int_0^{\pi}\sigma(\theta)\sin\theta d\theta d\phi \\ &= 2\pi\int_0^{\pi}\sigma(\theta)\sin\theta d\theta \end{aligned} \tag{4}$$

where we have already used the definition of the differential solid angle, $d\Omega = \sin\theta d\theta d\phi$. *Now plugging Eq. (3) in Eq. (4) we get,*

$$\sigma = \frac{2\pi}{k^2}\int_0^{\pi}\left[\sum_{l=0}^{\infty}(2l+1)\exp(i\delta_l)P_l(\cos\theta)\sin\delta_l\right]\times\left[\sum_{l'=0}^{\infty}(2l'+1)\exp(-i\delta_{l'})P_{l'}(\cos\theta)\sin\delta_{l'}\right]\sin\theta d\theta \tag{5}$$

For Legendre polynomials, we have the orthogonality relation:

$$\int_{-1}^{+1}P_l(x)P_m(x)dx = \frac{2}{2l+1}\delta_{lm} \tag{6}$$

Changing the variable of integration from θ *to* x *by defining* $\cos\theta = x$ *and using the orthogonal property of Legendre polynomials in Eq. (5) we have,*

$$\begin{aligned}\sigma &= \frac{2\pi}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)\exp(i\delta_l)\exp(-i\delta_{l'})\sin\delta_l(2l'+1)\sin\delta_{l'}\int_0^{\pi}P_l(x)P_{l'}(x)dx \\ &= \frac{2\pi}{k^2}\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)\exp(i\delta_l)\exp(-i\delta_{l'})\sin\delta_l(2l'+1)\sin\delta_{l'}\frac{2}{2l+1}\delta_{ll'}\end{aligned} \tag{7}$$

which finally reduces to,

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{8}$$

For $\theta = 0$, $P_l(1) = 1$ and the scattering amplitude is,

$$f(0) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\exp(i\delta_l)\sin\delta_l \tag{9}$$

The imaginary part of $f(0)$ is

$$\mathrm{Im}[f(0)] = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{10}$$

From Eqs. (7) and (10) we get the optical theorem,

$$\sigma = \frac{4\pi}{k}\mathrm{Im}[f(0)] \tag{11}$$

(2) Rutherford scattering: [10 pts] Consider the scattering of two particles through the potential

$$V(\mathbf{r}) = -\frac{ZZ'e^2}{r}e^{-\alpha r} \tag{12}$$

in the first Born approximation.

(a) Find the scattering amplitude, and express it in terms of the momentum transfer $\mathbf{q}$.

(b) In the limit $\alpha \to 0$, find the corresponding scattering cross-section. Why can we interpret this now as scattering through the Coulomb potential? Compare your result with the Rutherford scattering cross-section (e.g. PHY 106) and discuss.

Solution:
(a) In the first Born approximation, the scattering amplitude is (from Eq. (8.40))

$$f(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int d^3\mathbf{r}' e^{i(\mathbf{k}_{in}-\mathbf{k}_f)\cdot\mathbf{r}'}V(\mathbf{r}') \tag{13}$$

Inserting the value of the potential and taking $\mathbf{q} = \mathbf{k}_{in} - \mathbf{k}_f$, we get

$$\begin{aligned}
f(\theta) &= -\frac{m}{2\pi\hbar^2}\int r'^2 dr' e^{i\mathbf{q}\cdot\mathbf{r}'}\left(-\frac{ZZ'e^2}{r'}\right)e^{-\alpha r'} sin\theta' d\theta' d\phi' \\
&= \frac{ZZ'me^2}{\hbar^2}\int_0^{\infty} r'dr'e^{-\alpha r'}\int_0^{\pi} sin\theta' e^{iqr'cos\theta'}d\theta' \\
&= \frac{ZZ'me^2}{\hbar^2}\int_0^{\infty} r'dr'e^{-\alpha r'}\left(\frac{2sinqr'}{qr'}\right) \\
&= \frac{2mZZ'e^2}{q\hbar^2}\int_0^{\infty} sinqr'e^{-\alpha r'}dr' \\
&= \frac{2mZZ'e^2}{q\hbar^2}\frac{q}{q^2+\alpha^2}
\end{aligned} \tag{14}$$

with,

$$\int_0^\pi sin\theta' e^{iqr'cos\theta'} d\theta' = \frac{2sinqr'}{qr'}$$
$$\int_0^\infty sinqr' e^{-\alpha r'} dr' = \frac{q}{q^2 + \alpha^2}$$
$$q^2 = 4k^2 sin^2(\theta/2) \tag{15}$$

(b) In the limit of $\alpha \to 0$, $\frac{q}{q^2+\alpha^2} \approx \frac{1}{q}$.
In this case, the scattering amplitude is

$$f(\theta) = \frac{2mZZ'e^2}{\hbar^2} \frac{1}{q^2} \tag{16}$$

With the value of q^2 *from Eq. (15), the corresponding scattering cross-section is*

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{m^2 Z^2 Z'^2 e^4}{4\hbar^4 k^4 sin^4(\theta/2)}, \tag{17}$$

For $\alpha \to 0$, *the potential in Eq. (12) has the same form as the Coulomb potential and hence we can interpret the result in Eq. (17) as the scattering cross-section through the Coulomb potential,* $V(\mathbf{r}) = -\frac{ZZ'e^2}{r}$. *Thus the result in Eq. (17) matches exactly with the Rutherford scattering cross-section which is:*

$$\frac{d\sigma}{d\Omega} = \left(\frac{ZZ'e^2}{4E_k}\right)^2 \frac{1}{sin^4(\theta/2)} \tag{18}$$

if we plug $E_k = \frac{\hbar^2 k^2}{m}$ *in Eq. (18).*

(3) Two-dimensional scattering of wavepackets: [**8pts**] The code `Assignment5_2Dscattering_draft_v1.m` solves the TDSE in two dimensions

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y)\right]\Psi(x,y), \tag{19}$$

for the initial state

$$\Psi(x,y) = \frac{1}{(\pi^2 \sigma_x^2 \sigma_y^2)^{1/4}} e^{-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}} e^{ik_{\text{in}}x}, \tag{20}$$

and scattering potential $V(r) = A_{\text{pot}} e^{-r^2/\sigma_{\text{pot}}^2}$ with $r = \sqrt{x^2+y^2}$. The wavepacket is set up broad compared to the range of the scattering potential, so this is the closest we can get to the incoming plane wave discussed in the lecture, without having to worry about boundary conditions at the edge of the simulated domain in x and y.

(a) Run `Assignment5_2Dscattering_draft_v1.m` without changing parameters, and using the script `Assignment5_scattering_slideshow_v1.m` inspect the time evolution of the probability density $|\Psi(x,y,t)|^2$. Discuss what you see [3pts].
Solution: see caption of Fig. 1 below.

(b) Now, for various values of k_{in} in the range $k_{in} = 0.5..2$, run first the script `Assignment5_2Dscattering_draft_v1.m` to generate the evolution of the wavepacket without scattering potential $\Psi_{nsc}(x, y, t)$, and then `Assignment5_2Dscattering_draft_v1.m` with the same value of k_{in}, to generates the evolution with scattering potential $\Psi(x, y, t)$. Finally use `Assignment5_comparison_wfct_slideshow_v1.m`, which first calculates only the scattered part of the wavefunction $\Psi_{out}(x, y, t) = \Psi(x, y, t) - \Psi_{nsc}(x, y, t)$ and then plots the density of that, to analyse the results (see figures (2) and (3)). Comment on what you see and why you see it. [5pts] *Solution: see captions of Fig. 2 and Fig. 3 below.*

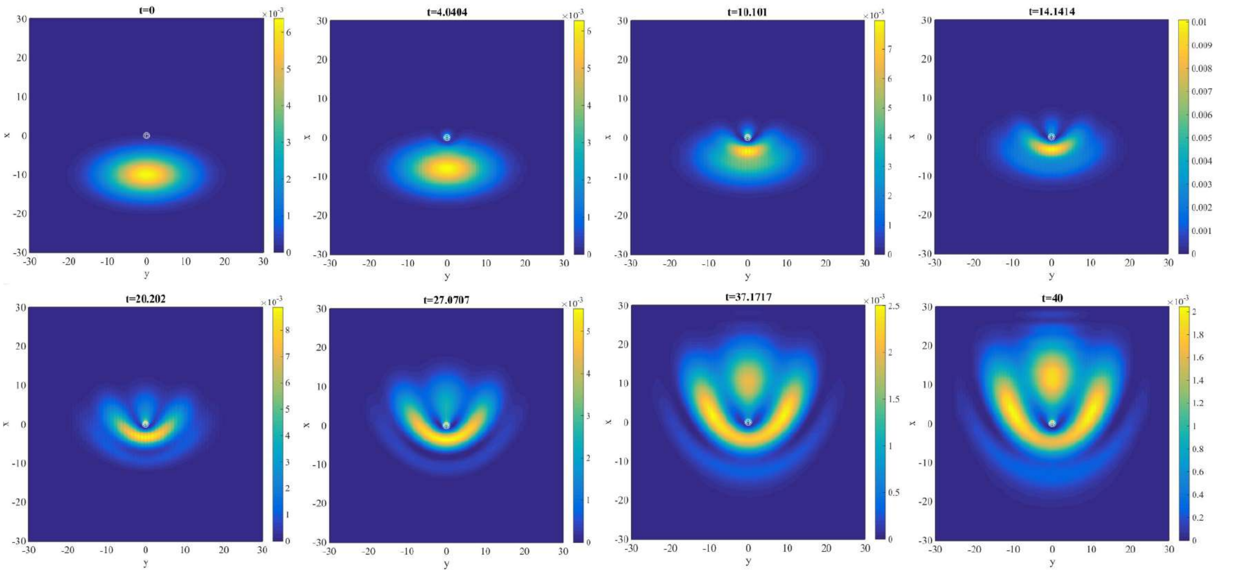

Figure 1: (**Q3(a)**) Time evolution of probability density for $k_{in} = 0.5$. We see that once the wavepacket hits the scattering potential, it becomes distorted and quantum interference features arise in the forward and in the backward direction. In the forward direction we see certain angles θ with high and some with lower probability density.

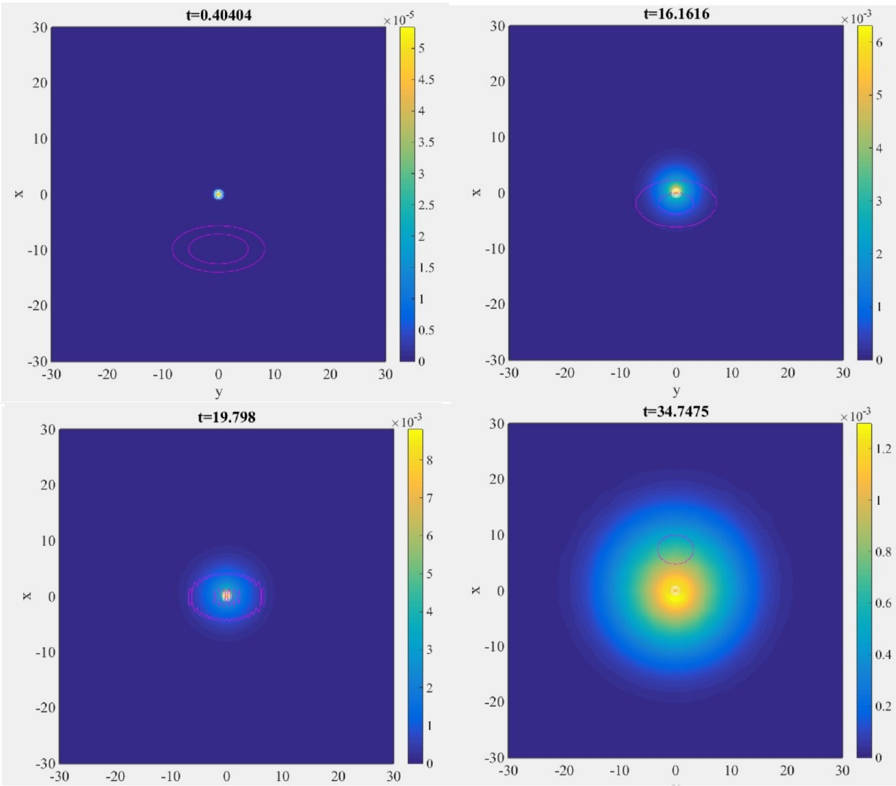

Figure 2: Time evolution of scattered part density $|\Psi_{out}(x,y,z)|^2$ for $k_{in} = 0.5$
The magenta circles indicate where the incoming scattering wavepacket would be (it is substracted out, in the construction of $\Psi_{out}(x,y,t) = \Psi(x,y,t) - \Psi_{nsc}(x,y,t)$). We see that, once it hits the scattering potential, a scattered wavepacket is created, that is going out in all directions spherically symmetric. We thus conclude that we are in the s-wave scattering limit, where the scattering amplitude f (density in a certain direction) is independent of the scattering angle θ. From our incoming wavenumber k_{in} we estimate $b_1 = 1/k_{in} = 2$ (see lecture notes), compared to a potential range of $R_{\text{pot}} = 0.7$ (from the code), hence $R_{\text{pot}} < 1/k$ and this makes sense. We also see that the outgoing part itself does not show any interference fringes. Those that we see in Fig. 1 are thus the result of interference between the incoming and outgoing waves.

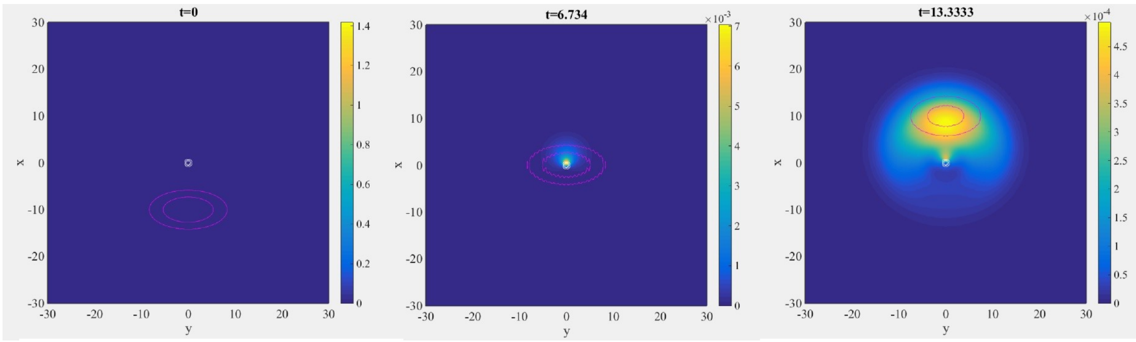

Figure 3: Time evolution of scattered part density $|\Psi_{out}(x, y, z)|^2$ for $k_{in} = 1.5$. Features are similar to Fig. 2, but for this higher scattering energy we have $b_1 = 0.6$ this has become quite close to the potential range of $R_{\rm pot} = 0.7$, hence we see an impact of p-wave scattering, with a typical $\cos theta$ dependence ($\theta = 0$ is in the direction of the incoming wavepacket's motion, hence up $(+x)$ in the figure, $\theta = \pi$ is down $(-x)$.