PHY 304, II-Semester 2023/24, Tutorial 6 solution

Stage 1 Wave scattering:

(i) Make drawing of 1D, 2D and 3D quantum scattering scenarios, and qualitatively discuss what degrees of freedom are there in the scattering wavefunction in each case, and which information is fixed by conservation laws. Does it make sense to talk about scattering in ND with $N > 3$?
Solution: See drawings in Fig. 1. Due to energy conservation we know the incoming and outgoing wavenumbers are the same, and we know the directions the outgoing wave can take. In 1D this is only two choices, left/right, in 2D any polar angle φ as shown, in 3D any two spherical polar angles θ and φ. The key unconstrained part of the process is "how likely" each outgoing direction is, i.e. R and T for 1D, or the scattering amplitudes $f(\varphi)$ in 2D or $f(\theta, \varphi)$ in 3D (note in the lecture we assumed a spherically symmetric potential, then the 3D result cannot depend on φ, but for other potentials it might).

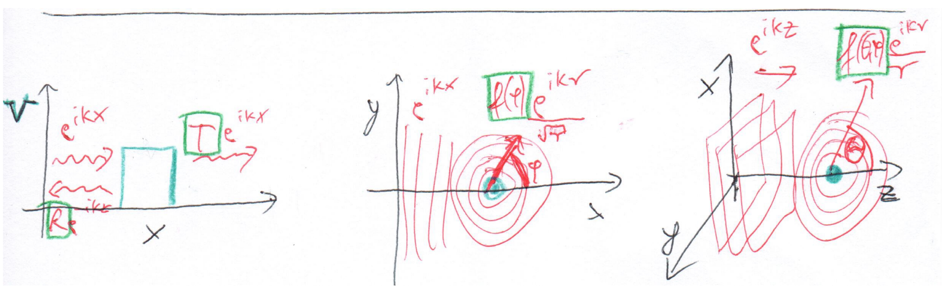

Figure 1: (**stage 2 (i)**) From left to right: Scattering in 1D, 2D, 3D. Red indicates waves (e.g. equal phase fronts for 2D, 3D). Cyan is the potential related to the target/obstacle. Green boxes encircle the crucial free information in the scattering process.

(ii) Discuss in your team the physical meaning (as opposed to mathematical definition), of "scattering angle“, "scattering amplitude", "differential cross section", "total cross section" and "partial wave amplitude".
Solution: See sections 8.1 and 8.2

(iii) Follow this link: https://physics.weber.edu/schroeder/software/ and then start the app "Quantum Scattering in Two Dimensions". Read the description, switch 'Barrier type" to "Circle" (or "Square"), and then do numerical experiments with sliders "Packet energy", "Strength", "Size", "Softness",to make contact with as many concepts from the lecture as possible. *[Important note: STOP the simulation once any wave hits the outer edge of the box, it becomes nonsense afterwards]*. Discuss whether and how you can see

- The structure of the scattering state (8.8) discussed in the lecture.

- Interference
- Momentum dependence of scattering
- Others?

You may get back to this applet after doing assignment 5Q3, which provides you with a very similar code.

Solution: We can use the app to see how the wavefunction evolves during scattering off the circular or square potentials, as shown in Fig. 2.

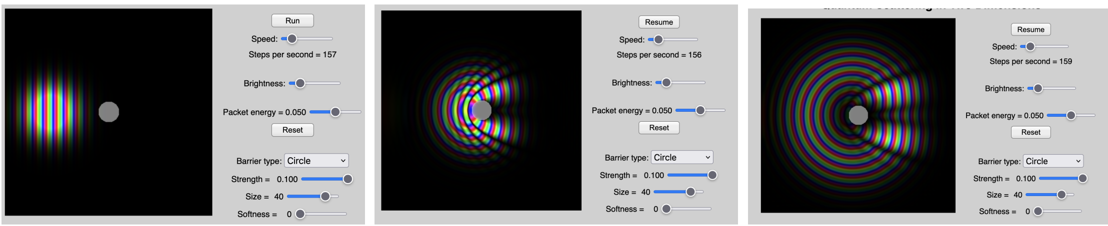

Figure 2: (**stage 2 (iii)**) Wavepacket (colored stripes) impinging on a circular potential (grey blob in centre). The colors in the wavepacket indicate the complex phase, thus the distance between two equal color stripes is the de-Broglie wavelength. (left) before scattering, (middle) during scattering, (right) after scattering.

One clearly sees that the outgoing scattering state is a radially outgoing wave. However in the forward half, there can be interference *between the incoming and the scattered wave. This causes the shape of phasefronts to be more complex. If we could run the simulation that long, we should check when the incoming and outgoing wavepackets are separated and would see a solely radially outgoing part and a rightmoving wavepacket, but before this could be seen, the waves hit the edge of the simulation box in the app. Another consequence of interference between incoming and outgoing wave are the low-amplitude minima, shown as curved dark regions in the froward direction, here those two contributions destructively interfere.*

To checkout the momentum dependence of scattering, we vary the "packet energy" setting of the app. Clearly the scattering behaviour is seen to depend on energy for this example where we have varied "softness" of the potential. For example the directions into which we have destructive interference are different in the three cases.

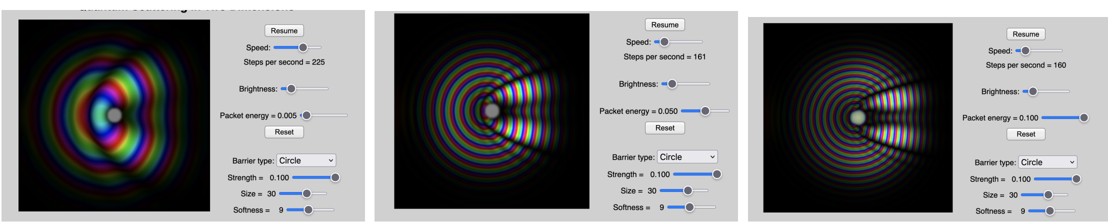

Figure 3: (**stage 2 (iii)**) The same style as Fig. 2 but for one scenario we show (left) low k/low energy, (middle) medium k/medium energy, (left) high k/high energy.

Stage 2 Partial wave expansion

(i) For the scenarios in Fig. 4, qualitatively discuss which partial waves ℓ you think might be significant and which angular dependence of the scattering amplitude f you would expect. Assume dimensionless units with $\hbar = m = 1$ and the following incoming wavenumber (momentum): (a) $k = 0.5$, (b) $k = 0.5$, (c) $k = 2$, (d) $k = 0.25$ and $k = 4$.

Solution: For each case, we make a drawing such as on page 202/ section 8.3.1 of the lecture notes, slicing the impact parameter plane up into slabs of a certain classical angular momentum as drawn below. For this we mainly have to calculate the slabsize $b_1 = 1/k$, which is (a,b) $b_1 = 2$, (c) $b_1 = 0.5$, (d) $b_1 = 4$ and (d') $b_1 = 0.25$. Roughly, we estimate the partial waves in slabs that include the potential (green) are relevant. For (a,b) this is $\ell = 0$ only (s-wave scattering). Regardless of potential shape, the angular dependence will thus be independent of θ ($Y_{00} = const$). For (c), from the picture, $\sim \ell = 0, 1, 2,$ might be relevant (note this is an estimate only, the quantum mechanical "slabs" are much less well defined, we can thus have an angular dependence of the scattering amplitude like $c_1 + c_2 \cos(\theta) + c_3 \cos\theta^2$ (from Eq. (8.18), and the fact that $P_{\ell=2}$ is a polynomial of second order.) (d) The $k = 0.25$ is again s-wave scattering, however at the higher scattering energy with $k = 4$ the potential range covers many angular moment and a quite complex θ dependence of the scattering amplitude f is possible.

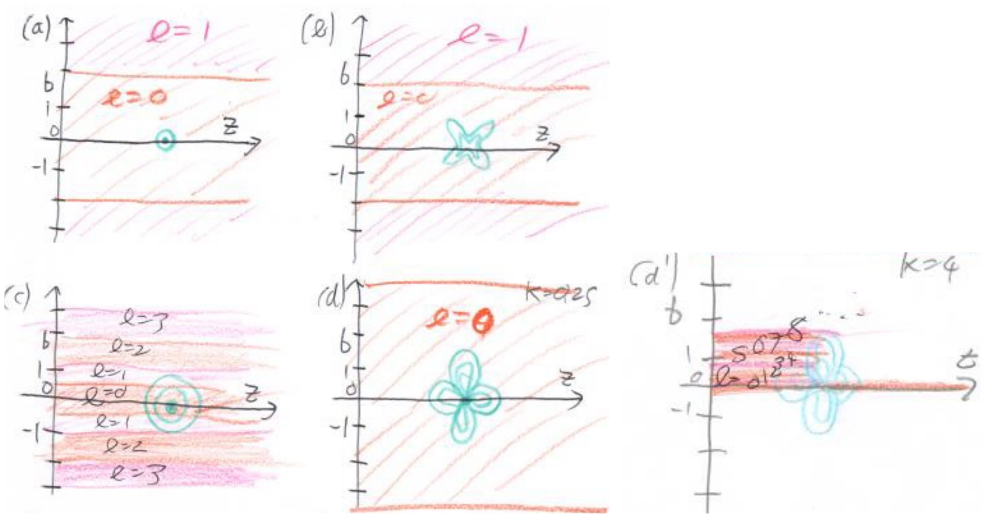

Figure 4: (**stage 1**) Scattering potentials $V(\mathbf{r})$ in the (b, z) plane as contour plots (green). We have added the angular momentum decomposition of the impact parameter plane in different colors, as discussed in the text.

(ii) Consider scattering at low energy E of a spherically symmetric square well potential $V(\mathbf{r}) = -V_0\theta(a-r)$ with $r = |\mathbf{r}|$, such that the radial TISE [Eq. (8.19)] in the $\ell = 0$ channel reads

$$\left[\frac{d^2}{dr^2} - V(r)\right] u_0(r) = -k^2 u_0(r), \tag{1}$$

and the solution can be written as

$$u_0(r) = \begin{cases} C \sin{(Kr)}, & r \leq a \\ \sin{(kr + \delta_0)}, & r > a. \end{cases} \tag{2}$$

with $k = \sqrt{2mE}$, $K^2 = k^2 + V_0^2$ and real δ_0. Discuss in your team first why/when looking at $\ell = 0$ only is justified, with which steps you can find the total scattering cross section and s-wave scattering length or s-wave scattering phase shift, all the way to the end. If there is time, then also perform those steps (in that case justify (2) first).

Solution: Discussion of steps: It is sufficient to look at $\ell = 0$ *only as long as the range of the potential (here* a*) is much less than* $1/k$*, with* $k = \sqrt{2mE}/\hbar$*. Let us assume that is the case. We can then solve Eq. (1) over all* r*, essentially doing regions (I-III) alltogether [e.g. region II is not required if we look at* $\ell = 0$*]. For this we have to use the right boundary conditions (see below). To extract the scattering amplitude we then compare our solution with Eq. (8.18) [partial wave expansion of the scattering wavefunction]. From this comparison we can determine (read off) the scattering amplitude* a_0 *or scattering length/phase shift.*

Execution of steps (Bonus): First we justify (2). The radial TISE (1) takes the exact same form as the 1D ones we had studied in QM-I section 2.2. on "piecewise continuous potentials". We split up space into regions I and III as shown in Fig. 5, skipping region II, such that our region numbering also is consistent with the one proposed in QM-II section 8.3.2. (partial wave expansion). We can write the general solution in both regions as

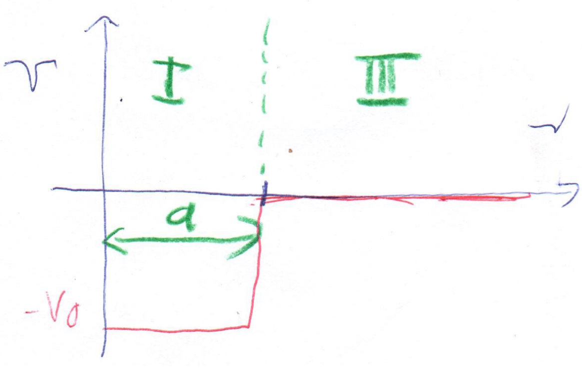

Figure 5: (**stage 1**) Radial potential $V(r)$ and regions I and III.

$$u^{(I)}(r) = A\cos Kr + B\sin Kr, \qquad \textit{for } 0 < a$$
$$u^{(III)}(r) = C\cos kr + D\sin kr, \qquad \textit{for } r > a, \tag{3}$$

using $k = \sqrt{2mE}/\hbar$ *and* $K = \sqrt{2m(E+V_0)}/\hbar$. *We know that the wavefunction and derivative must be continuous at* $r = a$ *since the potential has only a finite jump. Note that we do* *<u>not</u>* *have the boundary condition that* $\phi^{(III)}(r)$ *must vanish at large* r, *since we are looking at scattering states with* $E > 0$. *The remaining boundary condition to worry about is at* $r = 0$. *Suppose* $A \neq 0$, *then for small* r *we have*

$$\phi(\mathbf{r}) \approx \phi^{(I)}(\mathbf{r}) = \frac{u^{(I)}(r)}{r} \approx \frac{A\cos Kr}{r} \approx \frac{A}{r}. \tag{4}$$

From Eq. (8.33) we know that the 3D Laplacian applied onto $1/r$ *gives a delta-function, but there is nothing in the 3D TISE that can compensate it since the potential at* $r = 0$ *is finite, thus we require* $A = 0$.

In region III, we can combine the cos and sin terms into a phase-shifted sine, and skip the normalisation constant since we do not care about the overall normalisation factor of the solution. We thus finally reached the form:

$$u_0(r) = \begin{cases} C\sin(Kr), & r \leq a \\ \sin(kr + \delta_0), & r > a. \end{cases} \tag{5}$$

that was provided to you.

Now we continuously attach the wavefunctions on the shell $r = a$:

1) $u(r)$ *continuous:*

$$C\sin(Ka) = \sin(ka + \delta_0) \tag{6}$$

2) $u'(r)$ *continuous:*

$$CK\cos(Ka) = k\cos(ka + \delta_0) \tag{7}$$

Eq. (6) and (7) implies:

$$K\cot(Ka) = k\cot(ka + \delta_0) \tag{8}$$
$$\implies \tan(ka + \delta_0) = \frac{k}{K}\tan(Ka) \tag{9}$$

Using the identity $\tan(x+y) = \frac{\tan x + \tan y}{1 - \tan x \tan y}$ *we can now see that:*

$$\frac{\tan(ka) + \tan(\delta_0)}{1 - \tan(ka)\tan\delta_0} = \frac{k}{K}\tan(Ka) \tag{10}$$
$$\implies \tan\delta_0 = \frac{k\tan(Ka) - K\tan(ka)}{K + k\tan(Ka)\tan(ka)}. \tag{11}$$

In the low energy limit $ka << 1$ we use $\tan(ka) \approx ka$. This implies

$$\tan\delta_0 \approx \frac{k\tan(Ka) - Kka}{K + Kk^2 a\tan(Ka)} \approx \frac{k}{K}(\tan(Ka) - Ka) \tag{12}$$

In the last step above we simply disregarded k^2 term in the denominator. The phase shift is then given by:

$$\delta_0 = \tan^{-1}\left(\frac{k}{K}(\tan(Ka) - Ka)\right) \tag{13}$$

$$\approx \frac{k}{K}(\tan(Ka) - Ka) \tag{14}$$

[Bonus from here]: We have thus found the scattering phase shift and could turn that into a scattering amplitude using Eq. (8.31):

$$a_\ell = \frac{1}{2ik}\left(e^{2i\delta_\ell} - 1\right) = \frac{1}{k}e^{i\delta_\ell}\sin\delta_\ell. \tag{15}$$

The scattering length is $a_s = -f = -a_0$

$$a_s = -\frac{1}{k}\exp\left(i\frac{k}{K}(\tan(Ka) - Ka)\right)\sin\left(\frac{k}{K}(\tan(Ka) - Ka)\right) \tag{16}$$

$$\approx -\frac{1}{k}\left(\frac{k}{K}(\tan(Ka) - Ka)\right) \tag{17}$$

$$= \frac{Ka - \tan(Ka)}{K} \tag{18}$$

From Eq. (17) and (12) it can be seen that we could use the following equation which is taken really as the definition for scattering length:

$$a_s = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0 \tag{19}$$

To justify the use of above definition in another way, we recall scattering off a hard sphere. For a hard sphere of radius 'a', the scattering length is simply the radius of the sphere. i.e $a_s = a$. At $r = a_s$ then, the wavefunction must vanish, i.e. mathematically,

$$u_0(a_s) = \sin(ka_s + \delta_0) \tag{20}$$

$$= \sin(ka_s)\cos\delta_0 + \cos(ka_s)\sin\delta_0 \tag{21}$$

$$\approx \cos\delta_0(ka_s + \tan\delta_0) = 0 \tag{22}$$

For $\tan\delta_0$ we would only want terms of $\mathcal{O}(k)$. From Eq. (22 we then expect:

$$a_s = -\frac{1}{k}\tan\delta_0|_{with\ only\ \mathcal{O}(k)\ terms\ in\ \tan\delta_0} \tag{23}$$

Mathematically this can be written as:

$$a_s = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0 \tag{24}$$

You can check that the above equation gives $a_s = a$ for hard sphere. For any arbitrary potential we assume an effective radius or size of target a_s (which may not be equal to a) such that $u(a_s) = 0$. In this sense the scattering length provides an effective size of the target based on the scattering phase-shift.

The total scattering cross section is given by Eq. (8.22) of the lecture:

$$\sigma = 4\pi|a_0|^2 \tag{25}$$

where a_0 is the partial wave amplitude.

Since $a_s = -a_0$ we find total scattering cross section from Eq. (18)

$$\sigma = \frac{4\pi}{K^2}(\tan(Ka) - Ka)^2 \tag{26}$$

Note that for hard sphere of radius 'a', we would have expected $\sigma = 4\pi a^2$. For any arbitrary potential then, we simply replace 'a' by effective size or the scattering length giving $\sigma = 4\pi a_s^2$, which corresponds to Eq. (26).

Stage 3 Born approximation: Find the total scattering cross section for very low energy scattering from the potential

$$V(\mathbf{r}) = \begin{cases} V_0, & r \le a \\ 0, & r > a. \end{cases} \tag{27}$$

in the first Born-approximation.

Solution: We take the expression for the scattering amplitude in the first Born approximation (see Eq. (8.41) of the lecture) and simplify it even further taking $k \to$ on the RHS ("very low energy scattering"). This yields (see Eq. (8.45) of the lecture):

$$f = -\frac{m}{2\pi\hbar^2}\int d^3\mathbf{r}V(\mathbf{r}). \tag{28}$$

Since the potential is non-zero only within a sphere, and constant V_0 there, the result of the integral is that constant times the volume of the sphere $V_0 \times \mathcal{V}$ with $\mathcal{V} = \frac{4}{3}\pi a^3$, hence

$$f = -\frac{m}{2\pi\hbar^2}\left(\frac{4\pi a^3 V_0}{3}\right). \tag{29}$$

This gives us the total cross section from Eq. (8.22) of the lecture

$$\sigma = \int d\Omega|f|^2 = 4\pi\left(\frac{2mV_0a^3}{3\hbar^2}\right)^2. \tag{30}$$

Stage 4 Born series: Discuss in your team your intuitive understanding of the Born-series (or lack thereof, in which case try to get some).

Solution: See Eq. (8.49) and figure above example 68. The incoming plane wave may receive a local perturbation equal to the potential strength at all possible locations in space and all possible number of times. Each perturbation results in an outgoing (free) spherical wave (propagator). The final scattering wavefunction is the quantum mechanical superposition of all these possibilities.