PHY 304, II-Semester 2023/24, Tutorial 5

7. March 2024

Work in the same teams as for assignments. Do "Stages" in the order below.
Discuss on your table. When all teams finished a stage, make sure all students at your table understand the solution and agree on one by using the board.

Stage 1 WKB "approximation" for the particle in the square well potential

(i) Use Eq. (7.127) of the lecture (WKB wavefunction for the classically allowed region), to recover exactly the known solutions for the infinite square well potential [Eq. (2.10)] for allowed energies and corresponding wavefunctions. Why is it expected to get the exact result in this case?
Solution: We start with [Eq. (7.127)]:

$$\phi(x) = \frac{const}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int_{x_0}^{x} dx' p(x')} \tag{1}$$

For the case of the infinite well potential, the potential is zero inside the well, hence $p(x) = \sqrt{2mE}$ and we choose $x_0 = 0$.
We then have,

$$\begin{aligned} \phi(x) &= \frac{const}{\sqrt{2mE}} (C_+ e^{+\frac{i}{\hbar} \int_0^x \sqrt{2mE} dx'} + C_- e^{-\frac{i}{\hbar} \int_0^x \sqrt{2mE} dx'}) \\ &= \frac{const}{\sqrt{2mE}} (C_+ e^{+ikx} + C_- e^{-ikx}) \end{aligned} \tag{2}$$

where we have already evaluated the integral and put $\frac{\sqrt{2mE}}{\hbar} = k$.
Now applying the boundary conditions as usual:
$\phi(0) = \phi(L) = 0$
we get:
$C_- = -C_+$ *and* $kL = n\pi$ *(refer section 2.2.1 of QM1 lecture notes for more details)*
Fixing the normalization, the whole thing tidies up to the exact solution we already know from QM-I:

$$\phi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \tag{3}$$

We know that the WKB approximation works well for cases where the variation of the potential is small (over the range of one de -Broglie wavelength). For the given case, the variation is anyways zero since the potential is constant: $V = 0$ and therefore the WKB gives an exact answer.

We see how integrating the phase of the exponential for our constant potential already gives the ansatz we take for solving the infinite well potential exactly.

(ii) Discuss why you cannot use the WKB quantisation condition Eq. (7.145) here, and explicitly check that this would give you the wrong result for the energy.
Solution: We cannot use that condition, since it has been derived explicitly for wavefunctions extending from one classical turning point to the other, including the slight penetration into the classically forbidden region. Since there is no penetration into the region outside the box here, the formula is not applicable.
Proceeding as in the previous step:

$$\int_{x_1}^{x_2} dx\, p(x) dx \overset{here}{=} \int_0^a dx\, \sqrt{2mE}\, dx = \sqrt{2mE}a \overset{!}{=} \left(n - \frac{1}{2}\right)\pi\hbar, \tag{4}$$

hence

$$E_n = \frac{\left(n-\frac{1}{2}\right)^2 \pi^2\hbar^2}{2ma^2}. \tag{5}$$

Compared to the correct answer

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \tag{6}$$

we see that Eq. (5) is systematically shifted to lower energies. This systematic shift is because of the extra-delocalisation into regions outside the box, which is "assumed" by that formula, which lowers the kinetic energy.

Stage 2 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).

(ii) Discuss in your team the physical meaning (as opposed to mathematical definition), of "scattering angle", "scattering amplitude", "differential

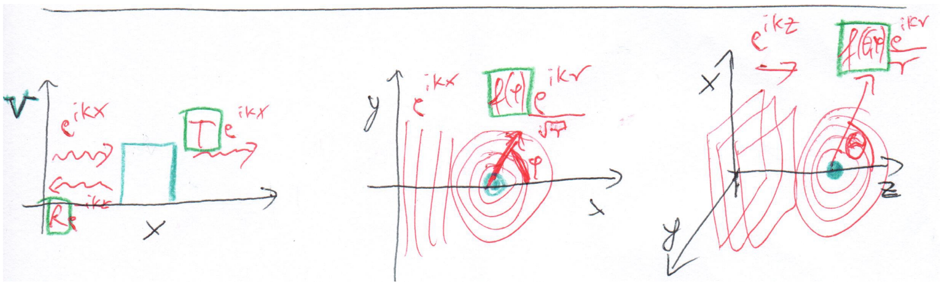

Figure 1: (**stage 2 (i)**) From left to right: Scattering in 1D, 2D, 3D. Red indicates waves (e.g. equal phase fronts for 2D, 3D). Cyan is the potential related to the target/obstacle. Green boxes encircle the crucial free information in the scattering process.

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.

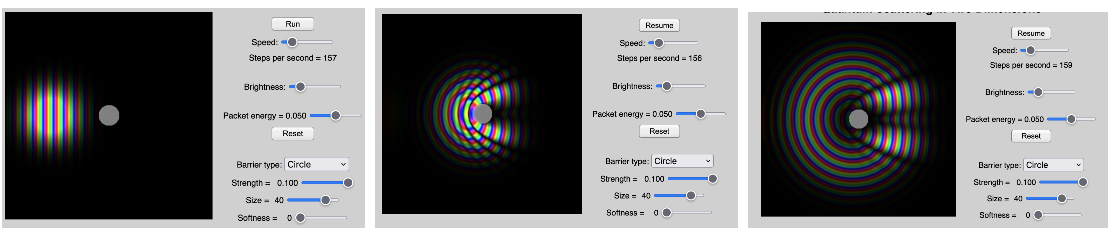

Figure 2: (**stage 2 (iii)**) Wavepacket (colored stripes) impinging on a circular potential (grey blob in centre). The colors in the wavepacket indicate the complex phase, thus the distance between two equal color stripes is the de-Broglie wavelength. (left) before scattering, (middle) during scattering,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

One clearly sees that the outgoing scattering state is a radially outgoing wave. However in the forward half, there can be <u>*interference*</u> *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.

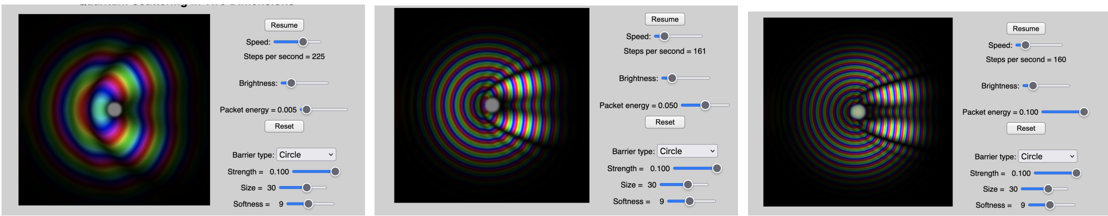

Figure 3: (**stage 2 (iii)**) The same style as Fig. 2 but for one scenario we show (left) low k/low energy, (middle) medium k/medium energy, (left) high k/high energy.

(iv) **Revisit mid-sem exam:** Lookat the mid-sem exam and do any question that you did not have time to do, or were not sure about. Only this time, it is open book and teamwork.

Stage 3 Revisit mid-sem exam: Look again at the mid-sem exam and do any question that you did not have time to do, were not sure about, or think you did badly. Only this time, it is open book and teamwork.

Solution: See mid-sem exam solution.