PHY 303, I-Semester 2023/24, Tutorial 3 solution

Stage 1 Particle in the box, online app: Start the online-app for exploring solutions of the TDSE at http://www.falstad.com/qm1d/ on your laptop or on a pad in AIR. Please go through the mini documentation `quantum_app_manual.pdf` provided on teams and/or the movie `quantum_app_manual.mp4` that I made, but ideally also read the more extensive online documentation.

We can now use this app to reproduce example 14 of the lecture. The default setting should be "setup: infinite well". There should be two white marked circles with rotating arrows at the bottom. These are the $c_{1,2}(t)$ from Eq. (2.19) represented in the complex plane. The height of the curve in the centre panel is $|\Psi_3(x,t)|^2$. The color shading indicates the complex phase $\varphi(x,t)$ of the wave function $\Psi_3(x,t) \equiv \sqrt{n(x,t)}e^{i\varphi(x,t)t}$. It turns out that lots of "color-stripes" indicate higher velocity, uni-color indicates small or no velocity.

(i) Inspect the eigenstates of the particle in the box, and qualitatively confirm all the results of the lecture, such as the dot-points below Eq. (2.18).

(ii) Now follow the instructions above to create Example 14 in the app. Discuss what you see. Look at the spatial variation of the phase, and interpret it in terms of a net velocity or probability current (see section 1.6.4.). How does this make sense intuitively?
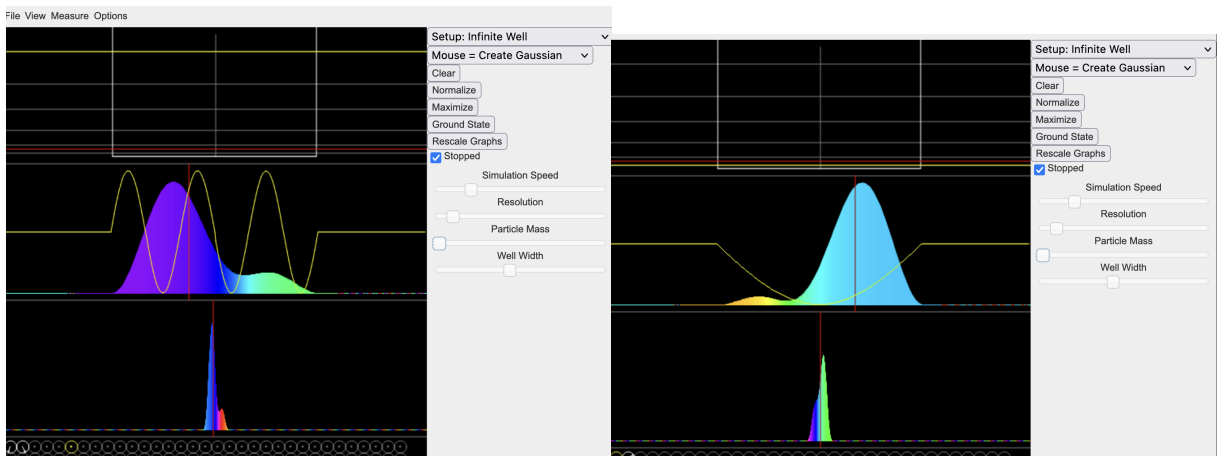

Figure 1: (left) Superposition similar to $\Psi(x,t=0) = \frac{1}{\sqrt{2}}\left(\phi_1(x) + \phi_2(x)\right)$. (right) Superposition similar to $\Psi(x,t>0) = \frac{1}{\sqrt{2}}\left(\phi_1(x) - \phi_2(x)\right)$.

Solution: See screenshots in Fig. 1 and compare with example 14. We also show sliderpositions so that you can recreate this scenario. We have created the superposition by clicking on the two first circular icons in the bottom left corner. As time proceeds, you see that the probability density is bouncing from right to left and back. This is consistent with the idea of the particle bouncing back and forth between the walls. The motion also shows up as phase gradient on the wavefunction (rainbow colors), compare Eq. (1.53)

and section 2.1. Also the phase gradient (and hence the underlying velocity) periodically changes direction. There has to be a probability current from right to left, if the probability density on the right is decreasing and on the left increasing.

(iii) Let us now combine the "particle in the square well potential' with a Gaussian wavepacket. Adjust all settings as shown in the screenshot below, and click with the mouse near the red-cross, which will create the wavepacket

$$\Psi(x, t = 0) = e^{i\frac{p_0}{\hbar}x}e^{-x^2/(2b^2)}/(\pi b^2)^{1/4}, \tag{1}$$

where p_0 is the momentum at which you have clicked into the panel near the red-cross. Discuss what the wavefunction means. Then discuss what you expect to happen. ONLY then, uncheck "stopped" and confirm your expectation with the simulation. Discuss the physical meaning of what you observe.
Solution: See screenshots in Fig. 2 and discussion in caption.

(iv) If the app did not exist, and you had to calculate the time-evolution from the given Gaussian initial state analytically, how would you proceed? *Solution: As in Quiz1, Q2(c), except that the initial state to be expanded would be Eq. 1 instead of the one given in Eq. (1) of that quiz.*

Stage 2 Harmonic oscillator, online app: Now switch the first pulldown menu to "harmonic oscillator".

(i) We want to reproduce example 16 (or assignment 2 Q2), on a classical looking oscillation using the app. For that, first create the ground-state of the oscillator. Then switch the second pulldown menu to "mouse, translate function", and move the ground-state gaussian a bit to the left or right. Then let it play. What do you see? You may also analyze <u>all</u> the panels in terms of our discussion of the Gaussian wavepacket and its Fourier transform in section 2.6.
Solution: See screenshots in Fig. 3 and compare with example 16 and Assignment 5 Q1.

(ii) In a slightly different approach, set the second pulldown menu to "mouse, create Gaussian", and click somewhere on the side from the centre of the oscillator potential. What is different to before? What is the same? Why do the differences happen? *Solution: See screenshots in Fig. 4. What is different, is that the Gaussian now also periodically changes its widths, while that had stayed constant in Fig. 3. What is still the same, is that it remains of Gaussian shape and oscillates left-right with the position expectation value (red vertical line in middle panel) performing a classical oscillation. The difference occurs because of the changed initial state width σ. Read also wikipedia "Squeezed coherent state".*

Stage 3 Quantum tunneling: The app also allows us to have a look at quantum tunnelling, but we have to "embed" the barriers within one of the potentials provided, such as a very large wide well.

(i) Change setup to "Well pair". You should see two square wells with a small barrier in between. This barrier is like the one discussed in section 2.2.4., except that here in the app, the space to the right and left is again limited by the far side of the square wells. Then select "Mouse = Create Gaussian" and click on the middle (wavefunction) panel into the right well. Discuss on your table what is happening initially and then after some time (30sec - 1 min). Interpret this with respect to section 2.2.4 lecture material. *Make sure the mass is the default value, else restart the app.*
Solution: See screenshots in Fig. 5.

(ii) Now use the sliderbar "mass" to increase the mass of the particle and do the above steps again. Increase 2-3 times. Then make it lighter than at the beginning. Discuss what you see. Is this consistent with Eq. (2.40)?

(iii) Use the slider "well separation" to vary the width of the barrier in the middle. Redo above steps. Discuss what you see and why.
Solution: With a bit of patience in this part, you should be able to qualitatively checkout the main dependencies of the transmission coefficient T (Eq. (2.38) and Assignment 3 Q2): T increases for lighter particles and decreases for wider or higher barrier potential. Since the dependence is exponential, it might be difficult to pick the right parameters to see the change without it directly jumping to 0.

Stage 4 Quantum Reflection: Getting the app to show quantum reflection is a bit tricky, but can be done.

(i) Change setup to "Coupled well pair". Click "stopped" to stop the animation. Then move sliderbar "well separation" all the way to the right, and sliderbar "mass" to just on the rhs of the word "mass". Switch the second pulldown menu to "create Gaussian" and click in the bottom most panel at the same horizontal position as the right edge of the barrier in the top panel.

The bottom panel shows you the Fourier-coefficients (momentum probability density), while the middle one shows you the position space probability density. The red line in the top most panel shows you the mean particle energy. Discuss in your group how you can see in these panels that we created the following initial state for the particle: It has an energy that is larger than the barrier energy $E > U_0$. It is initially most likely at $x = 0$ (in the middle of the screen) but moving to the right. *Solution: See screenshots in Fig. 6, here particularly for the position of slider bars. Note that the sequence that I got to work is a little different from the one suggested in the text.*

(ii) Now unclick "stopped" to start the simulation. If you are impatient slightly increase simulation speed. Discuss what happens once "the particle reaches the potential drop at the edge of the barrier".

(iii) What would you expect for a classical particle that we start on top of the barrier?

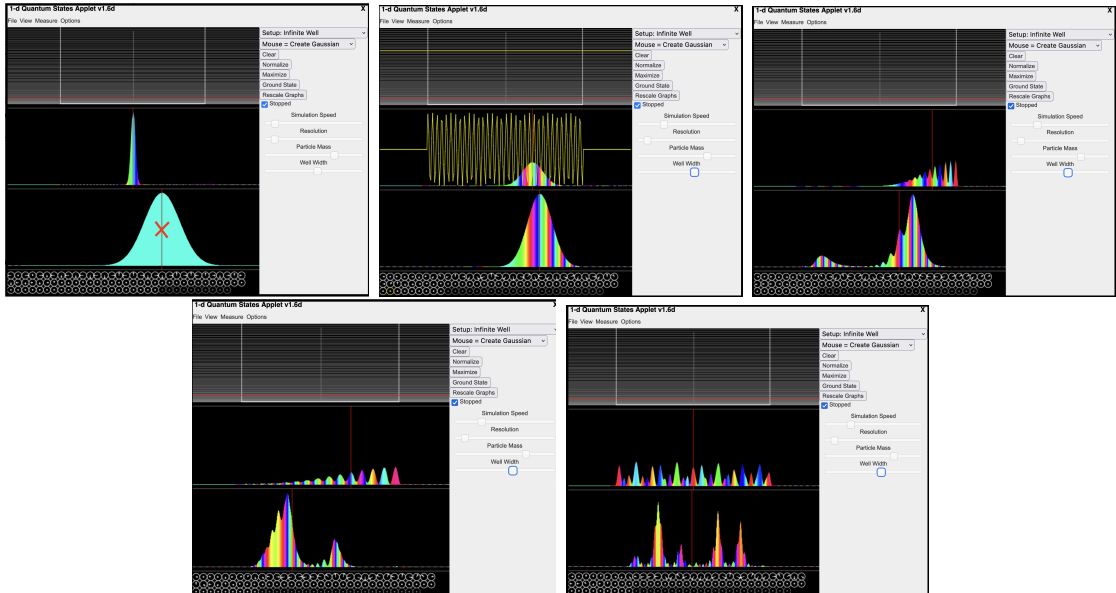*The classical particle would just keep going further, with 0 reflection probability.*

Figure 2: (top left) By clicking at the red cross, we have created a Gaussian wavepacket with nonzero mean momentum p_0 towards the right [bottom panel, where panel refers to the three pieces within EACH screenshot], in position space centered on the origin, [middle panel]. We can see that the particle is net moving to the right, since there is a corresponding phase gradient (color stripes) shown for the position space wavefunction $\Psi(x,0)$ in the middle row. (top middle) After a little while, the wavepacket has moved to the right as expected, and has also widened (see Eqs. (2.90) and (2.91)). (Top right) Once the particle hits the edge of the square well potential, it is elastically reflected since it has insufficient energy to escape. The reflected part shows up in the momentum probability density as a second peak on the left [bottom panel]. Simultaneously, the position probability density [middle row] now shows an interference pattern (small spaced spikes), between the parts of the wavefunction moving to the left and moving to the right. (bottom left) As time goes on, the probability of the particle already having been reflected increases, hence the left peak in the momentum probability density increases [bottom row]. (bottom right) After much longer times there will be a complex interference pattern in both position and momentum space.
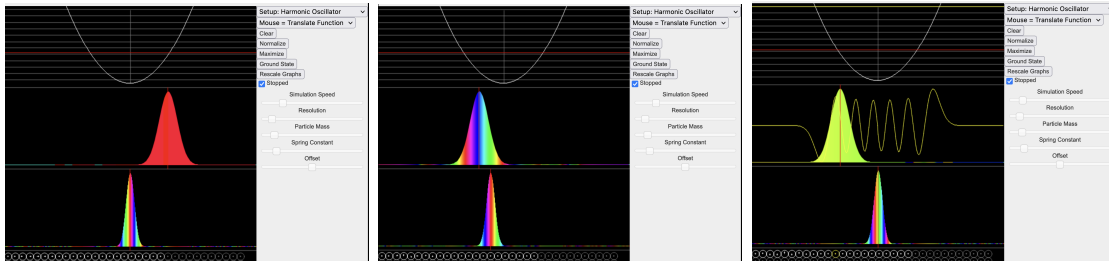
Figure 3: (left) At $t = 0$ we shift the Gaussian from the centre to the right. (middle) we see it starts moving to the left, while the wavefunction develops a phase gradient (rainbow colors) representing momentum to the left (right) At the turning point that phase gradient disappears for short when the particle comes to rest, then it begins moving back towards the right.
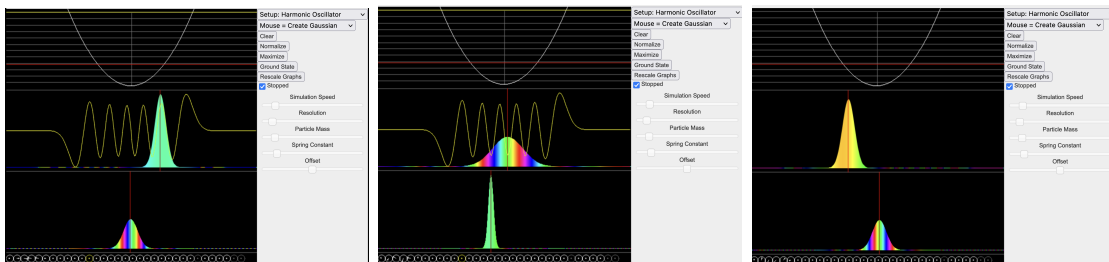

Figure 4: (left) At $t = 0$ we click on the right to create a Gaussian, but it ends up having a smaller width than the oscillator ground state. (middle) while moving to the left, this time it also changes width and spreads out (right) Just in time for reaching the turning point, it has narrowed down again.
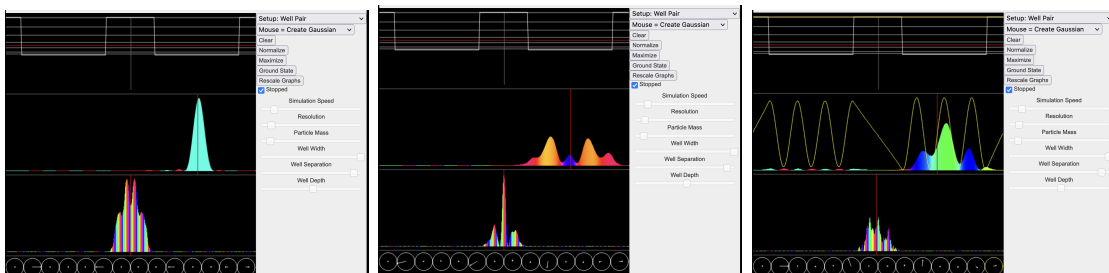

Figure 5: (left) The initially created Gaussian in the right well spreads (see section 2.6. and Eq. (2.90)) and hits the barrier (middle) For a while it seems that the particle is not able to penetrate the barrier and remains on the right (right) if we wait long enough, we see small non-zero probability density in the left well: a sign of quantum tunneling.
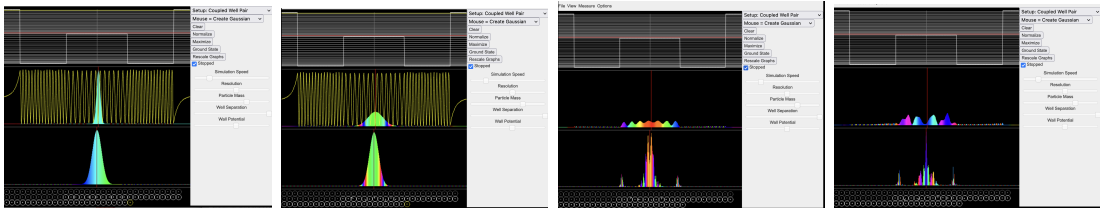
Figure 6: (left) The Gaussian is created in the centre of the barrier by clicking on the MIDDLE panel, not the bottom one (middle-left) It spreads as usual (middle-right) Once it hits the edge, you can see it reflected from the edge, even though the mean particle of the energy is higher than the barrier (red line in top panel) (right) If we wait long enough, small probability amplitude develops also in the well region, from that part of the wavefunction that was NOT reflected of the edge. Nontheless the particle remains trapped on top of the barrier with a very high probability.