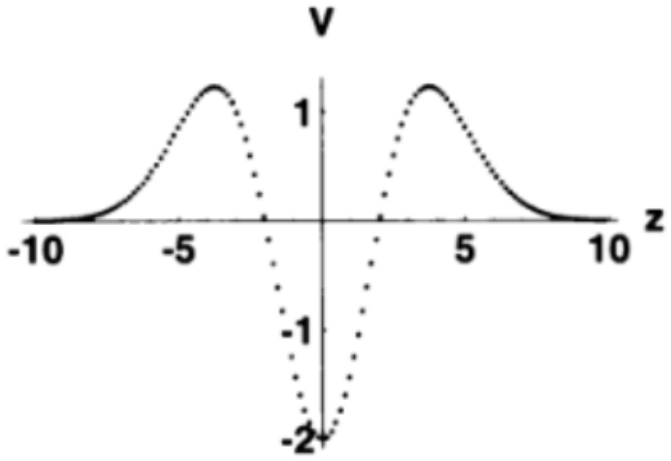
Problem

Investigate how an electron wave packet passes through a potential perturbation by performing numerical simulation. Does the wave packet take a longer time to emerge from the other side of the perturbation compared to the case of no perturbation? Use the potential profile given below, assuming the wave packet travels from the far left of the perturbed region to the right until it is sufficiently away from the region.



Reference: James M Feagin, Quantum methods with Mathematica, Ch. 14

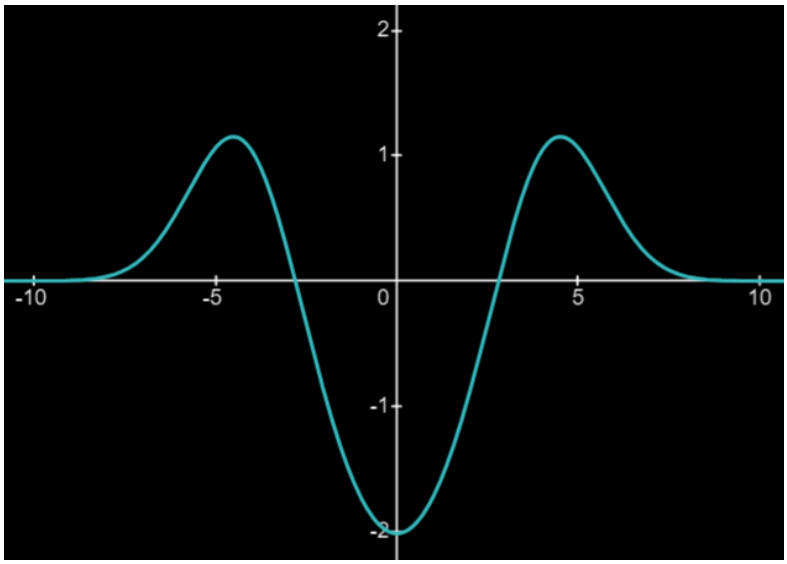
Solution

Summary of the problem: An electron wave packet goes through a non-zero (perturbed) potential. Compare the time it takes for the wave packet to pass through the perturbed versus the non-perturbed potential. Solve the problem via numerical simulation.

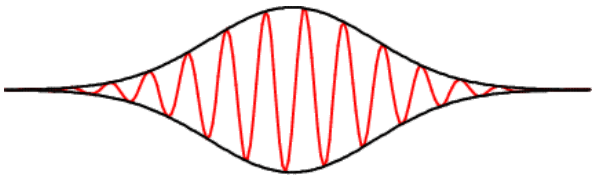
The function given is a potential energy vs position (z) function. The equation for the function is not given, so I have estimated it. The function shows two positive peaks around $x \approx 4.2$ and $x \approx -4.2$, where $y \approx 1.1$. It also shows a negative peak at $x \approx 0$, where $y \approx -2$. With this, we can presume that the function (via gaussian decomposition) is:

$$V(z) = 1.4e^{-\frac{(z+4.2)^2}{2^2}} + 1.4e^{-\frac{(z-4.2)^2}{2^2}} - 2.05e^{-\frac{z^2}{3^2}}$$

To clarify, I found these values by updating the function in Desmos to make it look similar to the problem. The potential looks like:



Now that the perturbed potential has been described, I can explain the electron wave packet. The red lines in the photo represent the underlying quantum wave, where the black represents a localized envelope.



The wave packet slides left to right along the potential. As the rightmost part of the wave packet hits the leftmost part of the potential function, the whole wave may be affected to keep the wave coherent. This is similar to pulling a blanket over your knees, where the whole blanket is affected. The electron wave packet represents the position of the quantum particle, where the center specifically represents the electron's average position. The spread of the wave packet represents the uncertainty in position. The oscillation speed within the envelope represents the electron's momentum.

The wave function can be represented by:

$$\psi(z,\ t)\ = \int A(k)\ e^{i(kz - w(k)t)}\, dk$$

For simplicity, we can represent the 1-Dimensional wave function at t = 0 as a gaussian:

$$\psi(z,\ 0)\ = e^{-\frac{(z - z_0)^2}{2\sigma^2}}\ e^{ik_0 z}$$

Here are some reasons we choose a gaussian:

- Localized in space
- Smooth while moving across a potential
- Well-defined average momentum
- "Easy" for numerical simulation (not computationally expensive)

Momentum-space amplitude is defined as

$$\psi(z,\ 0)\ = \int A(k)\ e^{-\frac{(z - z_0)^2}{2\sigma^2}},$$

Where our gaussian *A(k)* can be obtained numerically by taking the fast fourier transform of the initial wave packet.

$$A(k)\ = \mathcal{F}(\psi_0(z)).$$

This is also equal to

$$A(k)\ = \sigma\,(2pi)^{1/2}\ e^{-\frac{\sigma^2}{2}(k - k_0)^2}\ e^{-i(k - k_0)z}.$$

Finally, the 1-dimensional time-dependent Schrödinger equation can be defined by:

$$i\hbar \frac{\partial \psi(z,t)}{\partial t} = [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V(z)]\,\psi(z,\,t)$$

Where:

$$\hat{H}\,\psi = [\hat{T} + \hat{V}]\,\psi$$

We want to solve for the time evolution. To do this, we can treat the equation above as time-independent, solve for $\frac{\partial \psi(z,t)}{\partial t}$, and integrate from t to $t + \Delta t$, giving:

$$\psi(t + \Delta t) = e^{-\frac{i\hat{H}\Delta t}{\hbar}}\,\psi(t)$$

Ideally, we could just use this equation by plugging in the $\hat{T}$ and $\hat{V}$ operators. However, they don't share a basis because they act in different spaces. One acts on momentum space, while the other acts on position space. This can also be seen when showing that $[\hat{T}, \hat{V}]$ doesn't commute. To get around this, we can approximate by using the second-order Strang (symmetric) splitting method where

$$e^{-\frac{i\hat{H}\Delta t}{\hbar}} \approx e^{-\frac{i\hat{V}\Delta t}{2\hbar}} e^{-\frac{i\hat{T}\Delta t}{\hbar}} e^{-\frac{i\hat{V}\Delta t}{2\hbar}}$$

To clear confusion, I've added steps. $\hat{V}$ is diagonal in position space where:

$$\hat{V}\,\psi(z) = V(z)\,\psi(z)$$

So, we can apply the first $\hat{V}$ by multiplying terms by the wavefunction. Now we can apply a fast fourier transform to go into momentum space, thus defining $\hat{T}$ as diagonal, where we can say:

$$\frac{d^2}{dx^2} = -k^2 \quad \text{and} \quad \hat{T}\,\psi(k) = \frac{\hbar^2 k^2}{2m}\psi(k)$$

$\hat{T}$ can be applied by multiplying terms by the wavefunction. Then, we can inverse fast fourier transform back to position space and apply $\hat{V}$ again, where the final equation is:

$$\psi(t + \Delta t) \approx e^{-i\frac{V(z)\,\Delta t}{2\hbar}}\,\mathcal{F}^{-1}\left[\, e^{-i\frac{\hbar k^2 \Delta t}{2m}}\,\mathcal{F}\left(e^{-i\frac{V(z)\,\Delta t}{2\hbar}}\,\psi(z,\,t)\right)\right]$$

To determine the change in time, we start both the wave packets at the same point. This is roughly z = -100. The wave packet will travel across the potential. Once the wave packet's max ($|\psi|^2$) reaches z = 200, the timer is stopped. Essentially it's a drag race and we're testing which one is faster. Now that we've defined the problem conceptually, we can set up the simulation!

Symbol Representation:

z_0 = -100, initial center position

σ = 2, spatial width

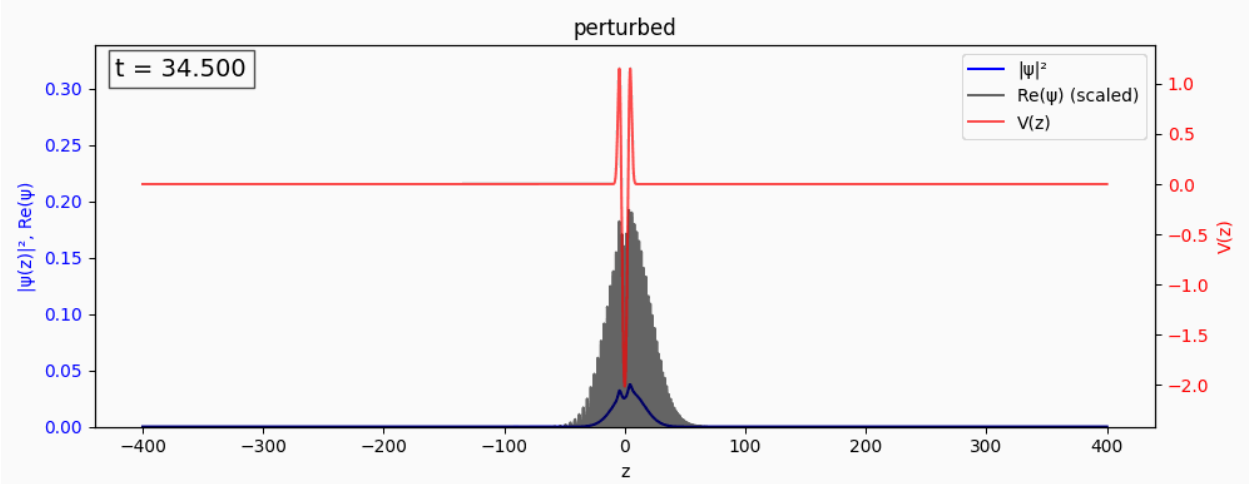
k_0 = 3, wave number, controls direction and speed of wave packet.

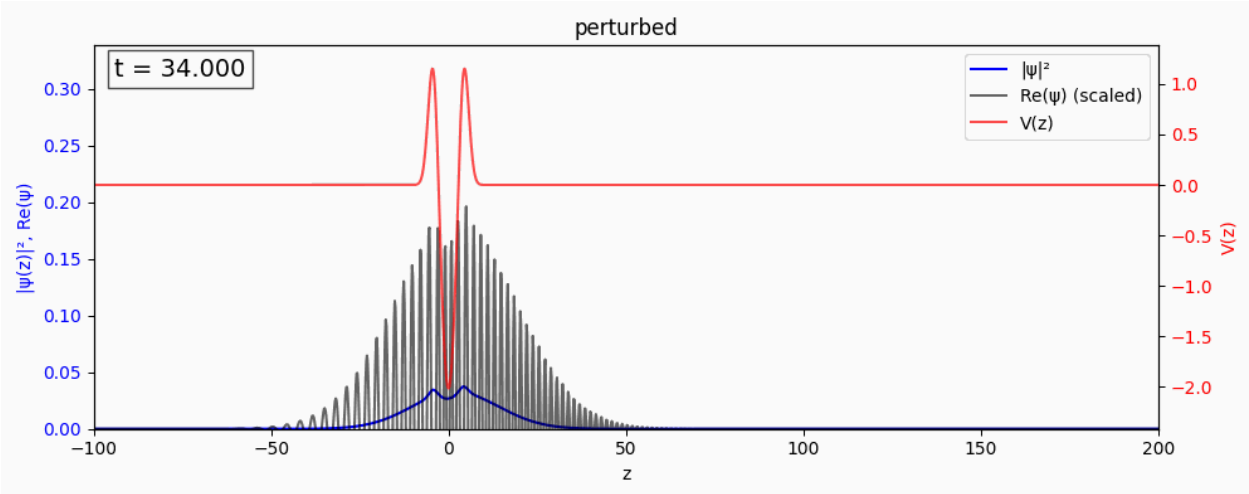
If σ is too small, the width is tightly localized and very spread in momentum. If it is too large, there is a small momentum spread. The wave number must also be large enough. Otherwise, part of the wave packet might not have enough momentum to overcome the bump potential, causing it to reflect backwards.

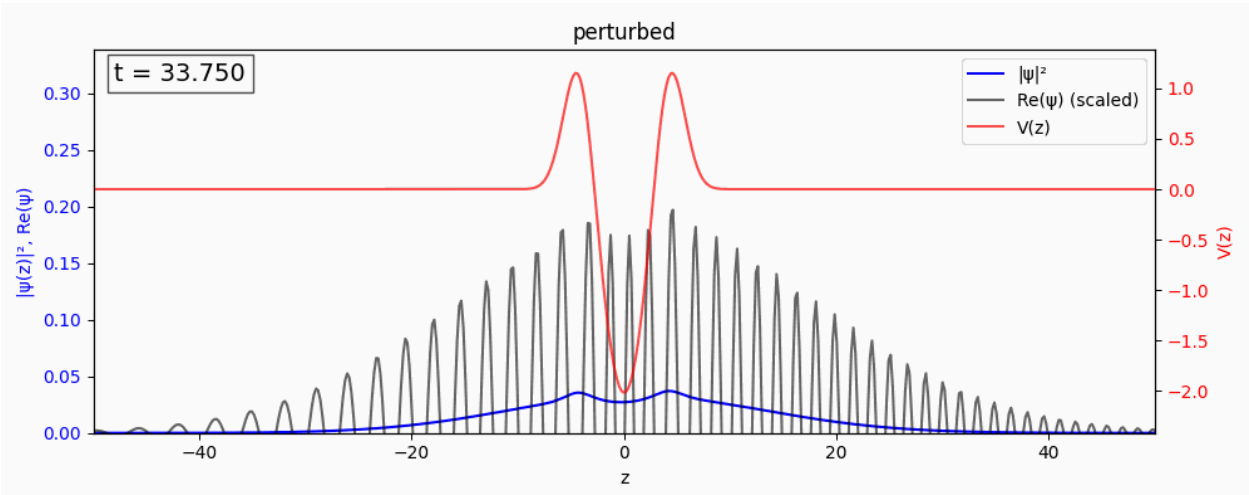
The general steps of the simulation are provided below:

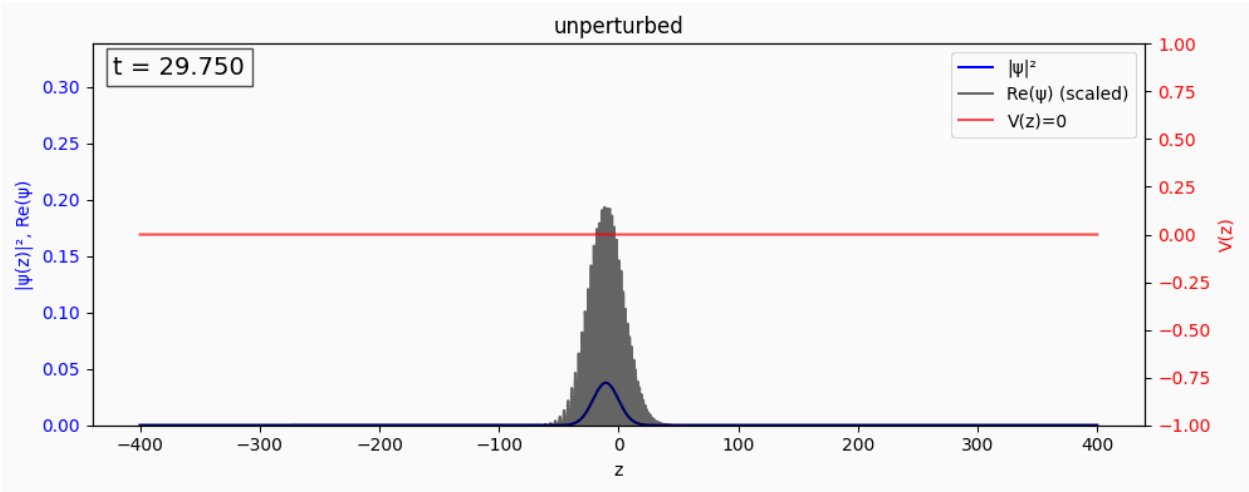
1. Make the spatial and momentum grids, import math, python, and other libraries
2. Define the basic parameters
3. Define the wave packet
4. Define the unperturbed and the perturbed potential
5. Define the split operator and respective functions to recall later
6. Define a "evolve" function to show how the wave packet changes over time
7. Run the simulation involving all the above
8. Plot a singular time step of the simulation
9. Re run the simulation and save pictures for all time steps
10. Use the pictures to create two gifs (one for perturbed and one for not-perturbed)

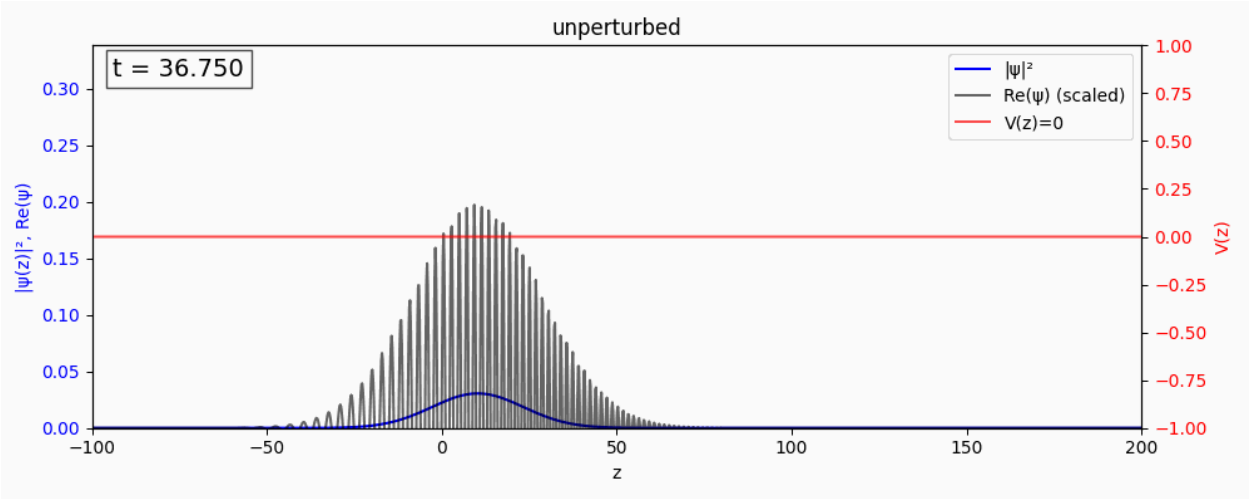
A few gifs will be shown during the presentation. However, screenshots of them are provided below. The first three photos are all a singular perturbed version, just zoomed in or out. They each show the potential (on a different axis) and the wave packet. Then, the last two photos are the unperturbed version. Finally, the physical bounds for the simulation are from [-400, 400] because if the bounds are too small, the wave does not freely propagate.


perturbed
t = 34.500
|ψ|²
Re(ψ) (scaled)
V(z)
|ψ(z)|², Re(ψ)
V(z)
z


perturbed
t = 34.000
|ψ|²
Re(ψ) (scaled)
V(z)
|ψ(z)|², Re(ψ)
V(z)
z


perturbed
t = 33.750
|ψ|²
Re(ψ) (scaled)
V(z)
|ψ(z)|², Re(ψ)
V(z)
z

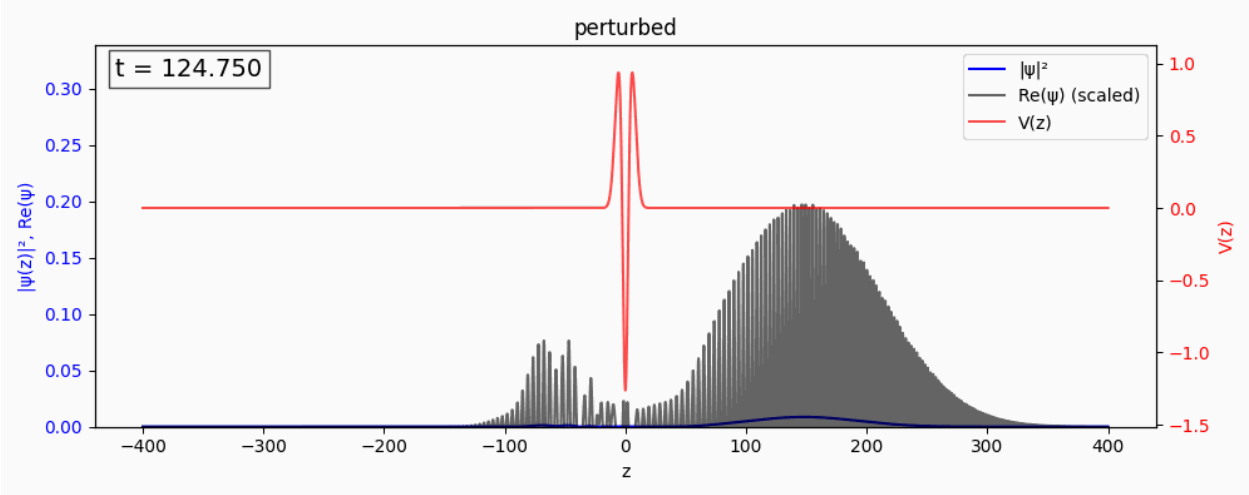




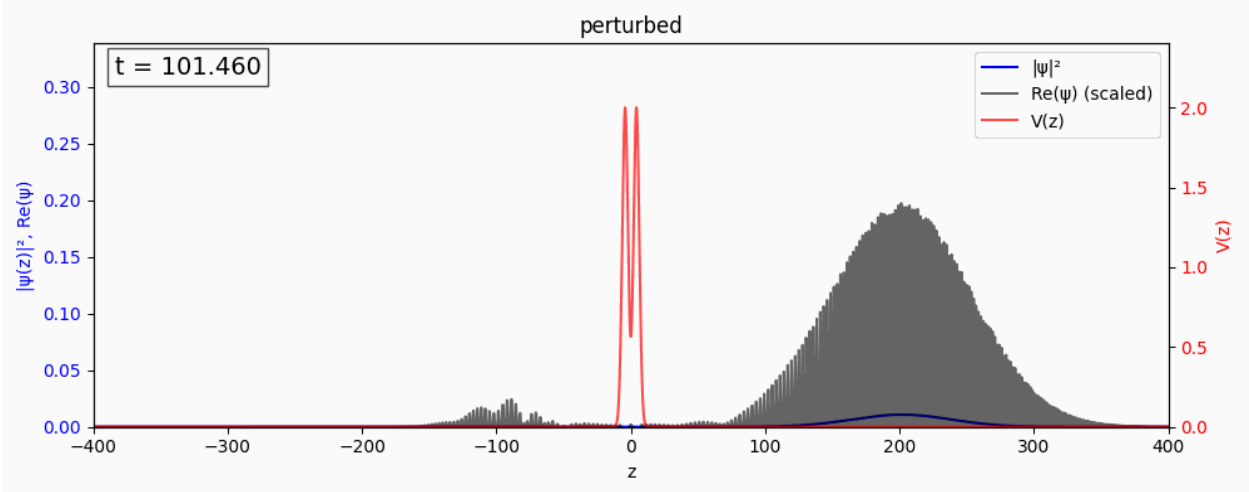
The perturbed version took 100.085 seconds and the unperturbed version took 100.005 seconds. The difference in time is 0.08 seconds.

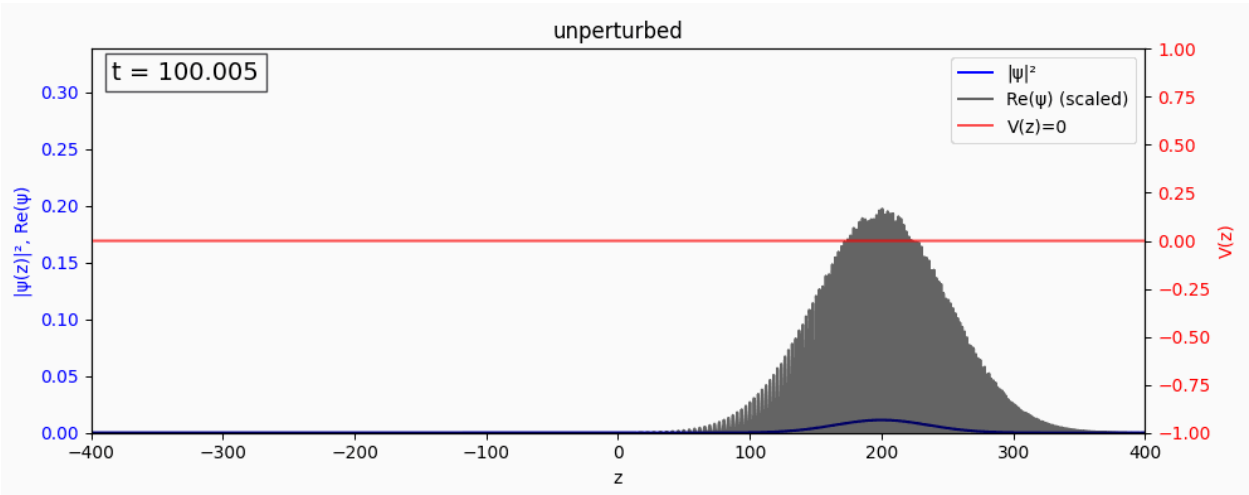
With an older version where the potential was not as exact, the difference in time was larger. As I refined the potential so that the total positive area and total negative area canceled out, the time difference decreased. Therefore, as the equation became more exact, the difference in time got smaller and smaller. This suggests that as the net area of the perturbation approaches zero, the wave packet experiences no delay.

Originally, I tested with a wave number of 2, rather than 3. However, I noticed that part of the wave packet didn't have enough momentum to overcome the wave packet. Here is what it looked like as it propagated.



I also ran a test under different parameters, but without the well and the time difference was 1.455 seconds. Here is that example:





The github repository to the code is: https://github.com/lhosk/wave-packet-pertubation/blob/main/perturbation_test.ipynb

References

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