

Figure 1. The propagation of a Gaussian wave packet,

$$\psi(x, t = 0) = \frac{e^{2ix - \frac{(x+10)^2}{16}}}{\sqrt{2}\sqrt{\pi}\sqrt{2}}$$

with known solutions. Final wave packet produced is $\psi(x, t = 10)$. The theoretical final

$$\psi(x, t = 10) = \frac{e^{-\frac{(x_{\text{values}} - x_0 - \frac{\hbar k_0 t}{m})^2}{2\sigma_t^2}}}{\sqrt{2}\sqrt{\pi}\sigma_t}$$

wave packet is,

. For small time steps the final wave packet closely matches the theoretical final wave packet. Percentage difference between the final wave packet and expected: 0.03250615450089471%.

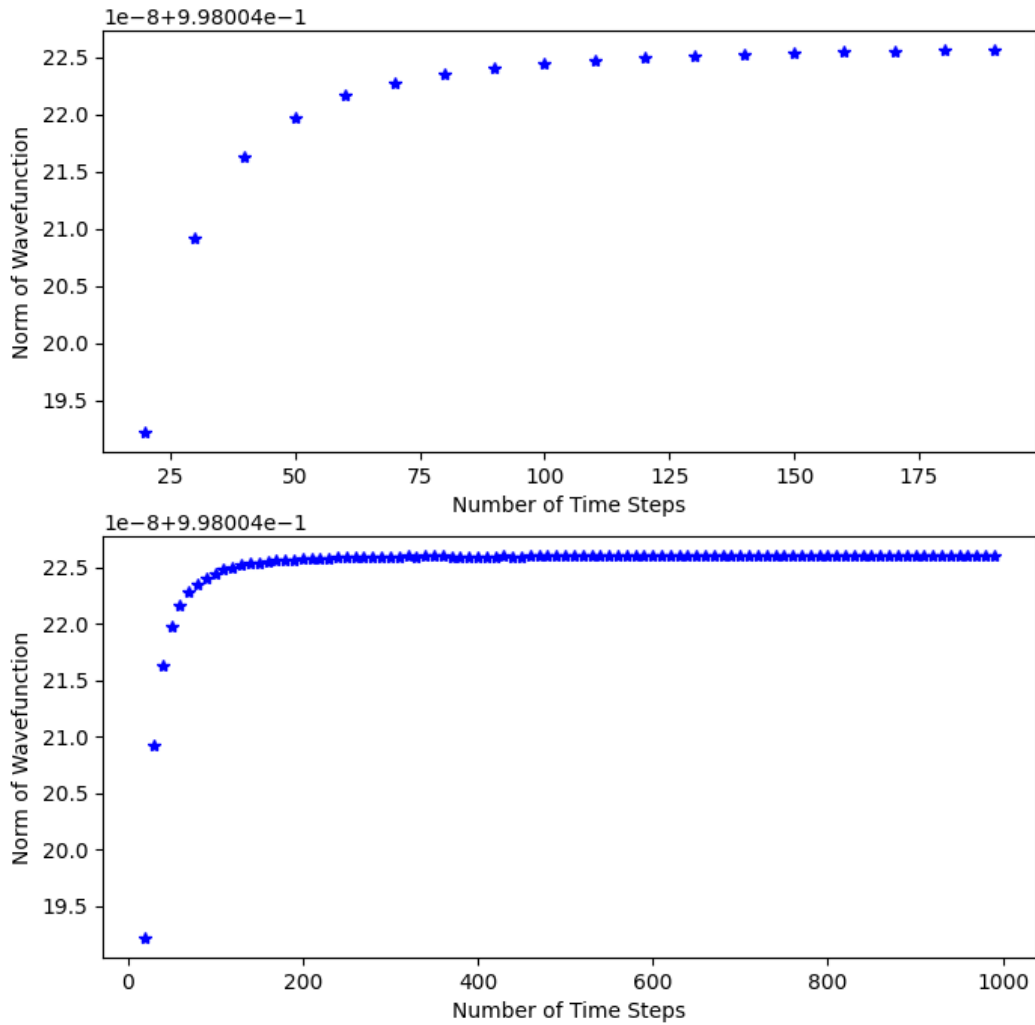


Figure 2. This graph shows how increasing the number of time steps, in the ODE calculation, makes the norm of the resultant wave function, $\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx$, closer to 1. Therefore, the higher the number of time steps, the better the validity of the results. The plot produced has an asymptote on the y-axis at $y=1$. This means that a lower time step can be used with very similar results, meaning that less computational power is needed for roughly the same error in calculation (useful for complicated problems). It is important to look at the scale of the y-axis, as each norm of each wave function is very close to 1.

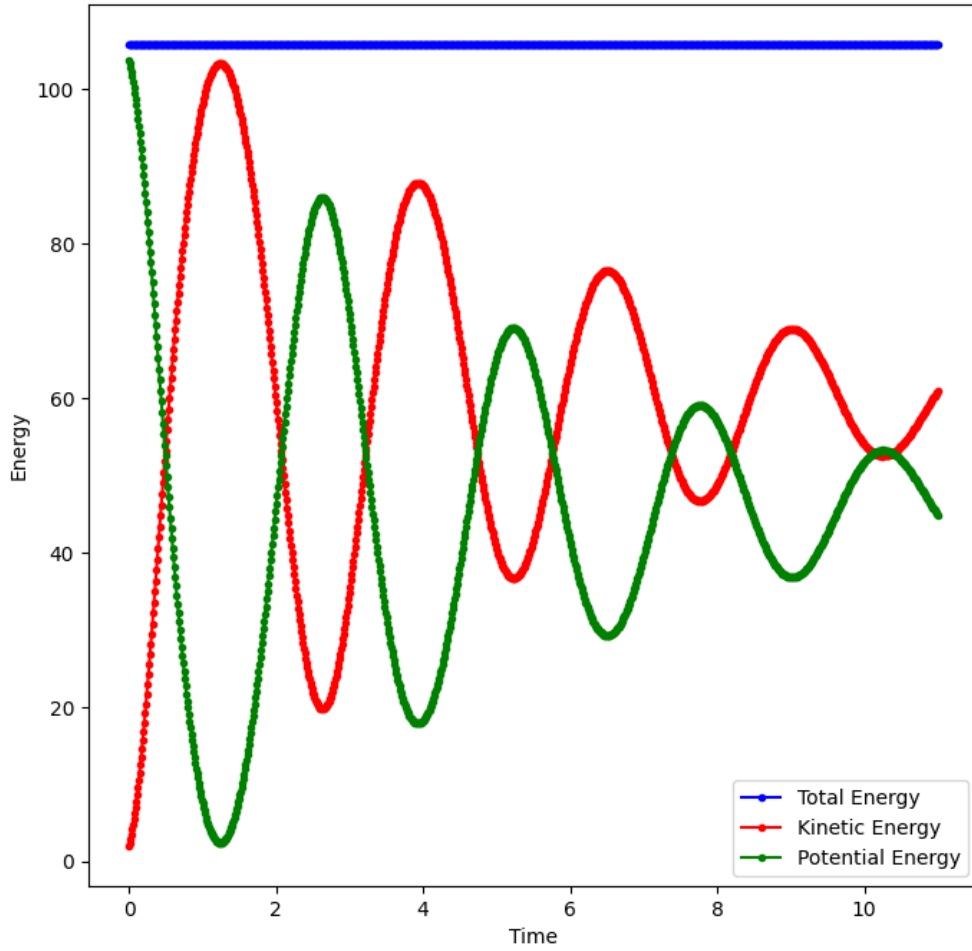


Figure 3. The above graph shows a Gaussian wave packet propagating through a Harmonic Potential of the form $V(x) = x^2$. Here $\langle \psi | \hat{T} | \psi \rangle$ & $\langle \psi | \hat{V} | \psi \rangle$ are constantly changing. However $\langle \psi | \hat{H} | \psi \rangle$ appears to remain constant. This agrees with the underlying physics of the system as total energy is conserved. When looking more quantitatively, it is seen that for the simulation of this particular system, there is a percentage loss in energy of the wave packet of 7.185983475612465e-05%. Therefore, the model works to conserve energy very well.

$$\psi(x, t = 0) = \frac{e^{2ix - \frac{(x+10)^2}{16}}}{\sqrt[4]{2}\sqrt[4]{\pi}\sqrt{2}}$$

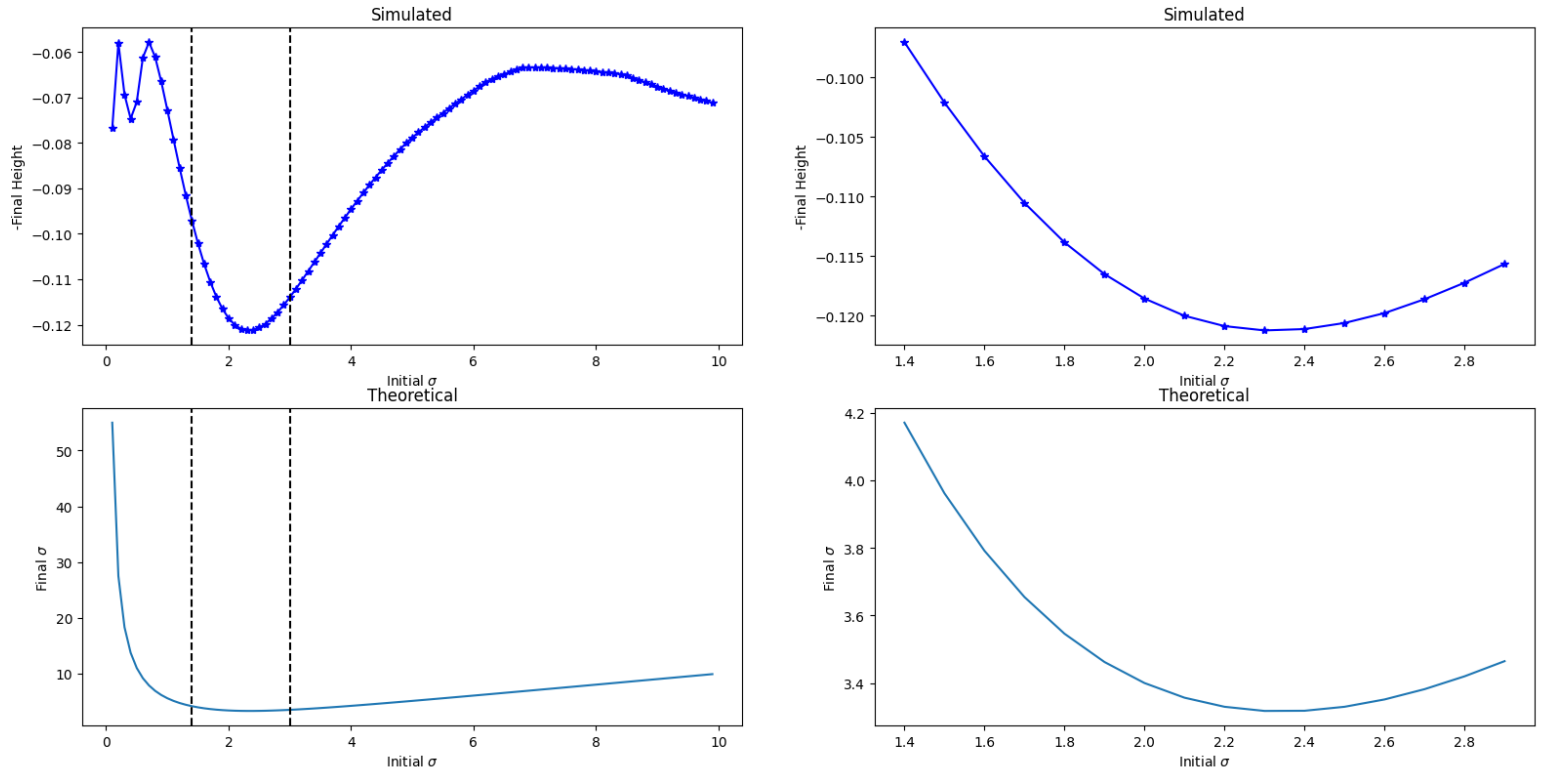


Figure 4. (fig.4a = top left, fig.4b = top right, fig.4c = bottom left, fig.4d = bottom right)
Demonstrates how varying the value of σ of the initial wavefunction,

$$\psi(x, t = 0) = \frac{e^{2ix - \frac{(x+10)^2}{16}}}{\sqrt{2}\sqrt{\pi}\sqrt{2}} = \frac{e^{-\frac{(x-x_0)^2}{4\sigma_0^2}}}{(2\pi)^{\frac{1}{4}}\sqrt{\sigma_0}} e^{ik_0x}, \text{ affects the final } \sigma \text{ value of the wavefunction}$$

at $t=11$. Expected $\sigma(t) = \sigma_0 \sqrt{\frac{(1+t^2)}{4\sigma_0^4}}$. This graph also demonstrates how the simulation breaks down for small σ and large σ , this can be seen qualitatively by the fact that fig.4a and fig.4c should be proportional. The breakdown of the simulation is due to how space is being discretised: for small σ , space does not have small enough steps and for large σ , there are not enough allowed x values, so the wavefunction goes over the barrier of allowed x values. However, for σ in between 1.4 and 3, the simulation holds. fig.4b shows that small σ waves spread out faster and for σ values above ~ 2.3 , the waves spread out slower for larger sigma. This matches the theoretical case shown in fig.4d, and proportionality holds.

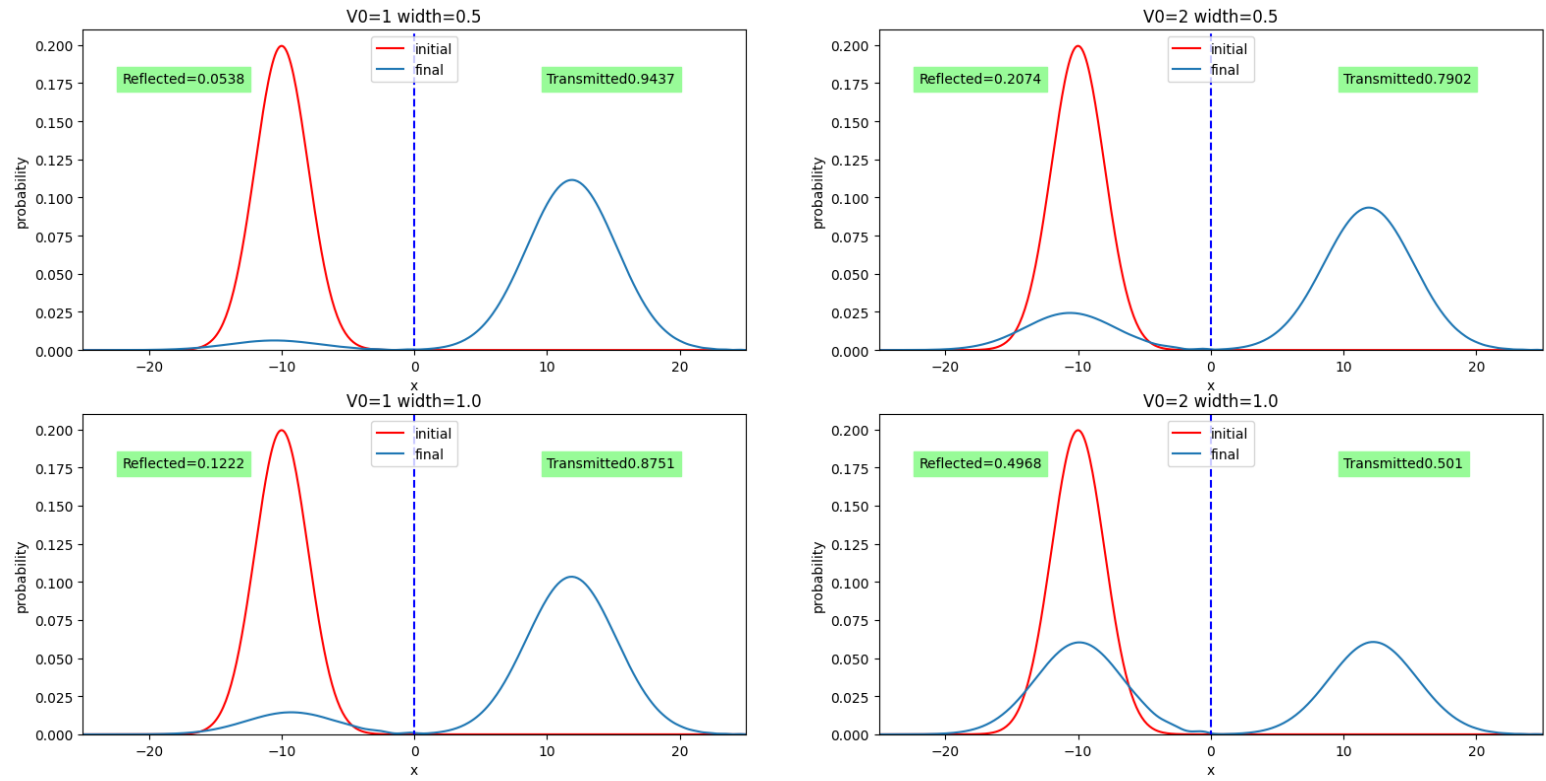


Figure 5. Each of the above plots demonstrate a Gaussian wave packet,

$$\psi(x, t = 0) = \frac{e^{2ix - \frac{(x+10)^2}{16}}}{\sqrt{2}\sqrt[4]{\pi}\sqrt{2}}$$

, propagating through particular rectangular potential barriers, outlined in the title for each plot in the figure. Each potential starts at $x=0$, with height= V_0 and width shown in title. The graphs show how changing the width and height of the potential changes the probability that a wave packet will tunnel through the rectangular potential barrier. It shows that increasing the height of the potential decreases the probability of tunnelling, and that increasing the width similarly decreases the probability of tunnelling. If you increase both variables simultaneously these effects are compounded. This is what is expected analytically.

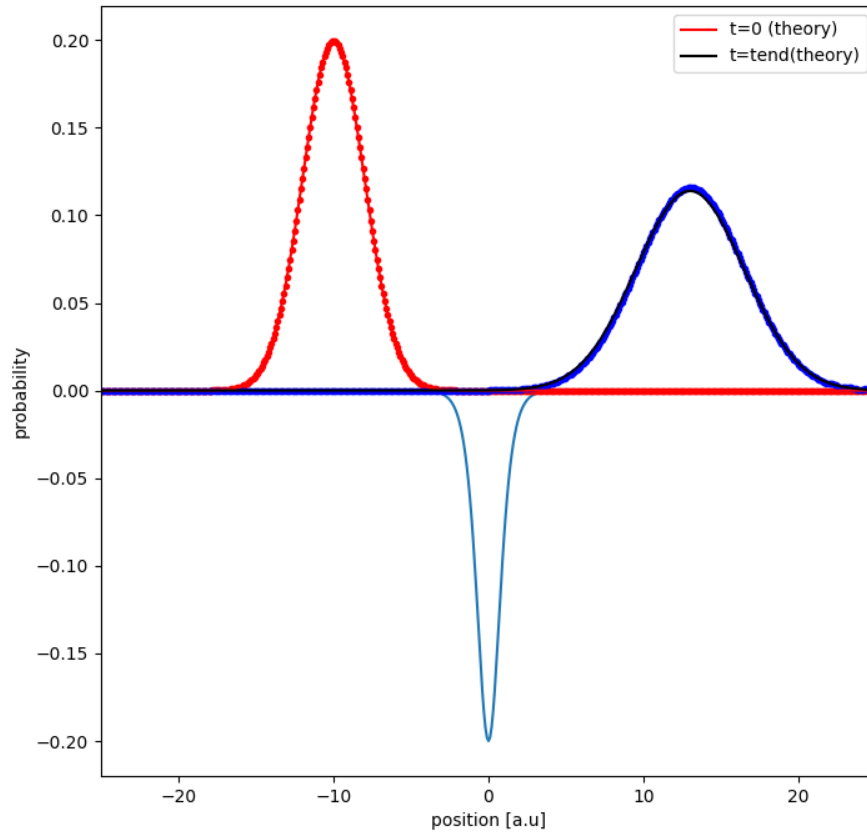


Figure 6. The potential shown above, $V(x) = -\frac{a^2 \hbar^2 \text{sech}^2(ax)}{5m}$, is demonstrated to be reflectionless, as the final wave packet matches the theoretical propagation of a free wave packet. Percentage difference between the simulated final wave packet and analytically expected free wave packet propagation: 0.035382577206373986%.

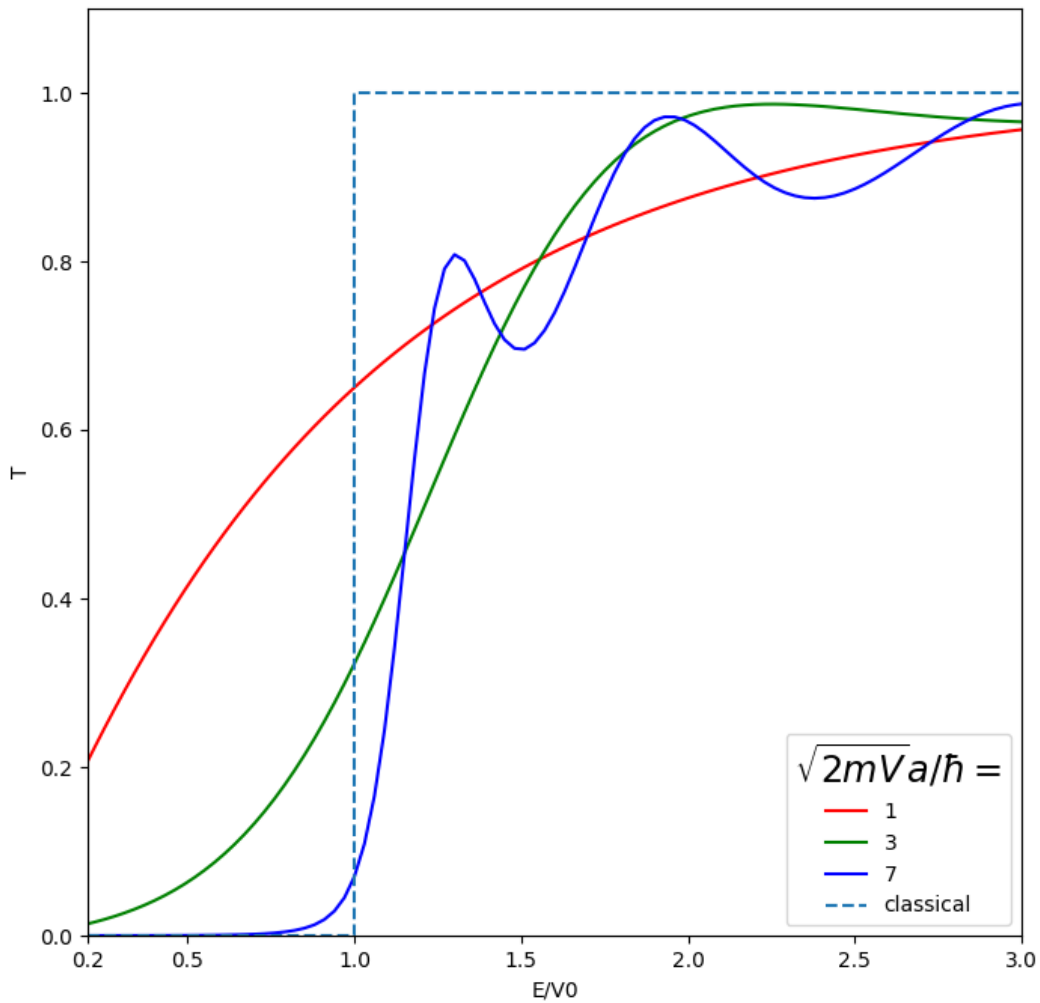


Figure 7. Transmission probability through a finite potential barrier for the values detailed in the legend. This figure shows how quantum tunnelling works in comparison with the classical case. For $E < V_0$, in the classical case transmission probability is equal to zero. However, in the quantum case, some transmission occurs, and less so for greater widths of potentials as expected. For $E > V_0$, in the classical case transmission probability is equal to one. However, in the quantum case, some reflection occurs. x-axis cuts off at 0.2, as low energy wave packets require too many time steps to compute within the confines of the computational power of the computer being used. However, from theory, all plots tend to 0 as E/V_0 tends to 0.