Time Delay in Near-Threshold Tunneling

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Abstract

We did theoretical analysis of time dependence in systems with a particle incident on a potential barrier with a maximum potential very close to the energy of the particle. Based on numerical computer models from the 1960s, we hypothesized a delay effect in which time spent under the potential increases rapidly as the energy approaches the peak of the potential. To analyze this effect, we calculated the Wigner time of an incident Gaussian wave packet reflecting against various soluble potentials. Analysis showed such a delay proportional to $\frac{1}{\sqrt{1-E}}$ for reflection from a step potential, which diverges at the threshold energy. This delay seems to persist for all analysis of a tanh potential. In the near future we additionally want to solve for square and sech potentials, as well as a general smooth potential with the WKB approximation. The results of this analysis could be relevant to any system with a classical turning point.

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1 Introduction

In the 1960s, Judah Schwartz and his team at MIT did a simulation of a tunneling particle on a primitive computer system. Specifically, he was simulating wave packets incident on square barriers of various potentials. Although the wavefunctions of much lesser and much greater energies behaved predictibly, reflecting or transmitting with negligable delay, as the energy approached the potential it started behaving differently. Part of the wavefuncion remained under the potential for long periods of time. When Schwartz gave a talk on the subject, in attendance was Eugene Wigner, a giant in the field of quantum tunneling. He found this effect intriguing. He has done work on similar problems, including developing the Wigner time, a method of following the peak of a wave packet which we are using now to measure the travel time. Although Schwartz mentioned this holding behavior in a 1967 paper[1] on computer simulation, he never published anything specifically about it and the subject stagnated. Very recently, he gave another talk at Tufts, and lamented that very little work had been done regarding this strange effect. We have now explored this strange effect in greater detail, specifically examining step and tanh potentials and beginning analysis on a general smooth potential with the WKB approximation.

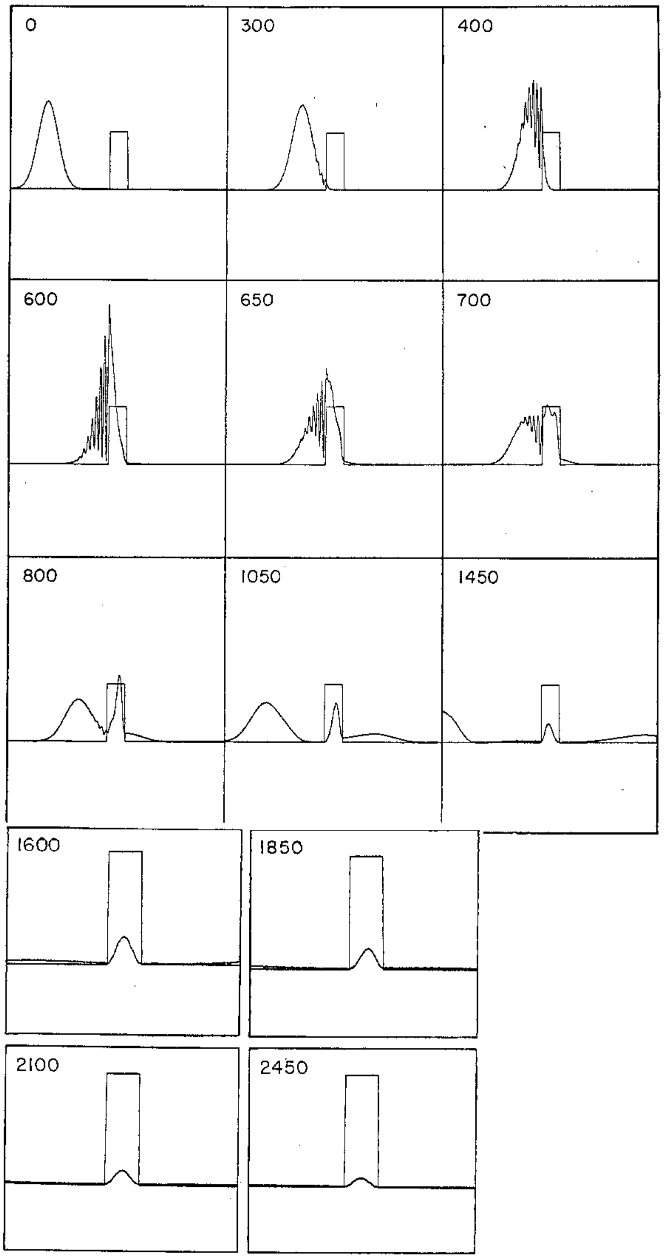

Figure 1: Schwartz' time-resolved movie of a wavefunction of energy equal to the potential barrier. Note the piece of the wavefunction remaining under the potential.

2 Applications

This research could have some fairly important implications. Photons are roughly analogous to wavefunctions, despite having two time derivatives in their characteristic equation rather than one, and could therefore exhibit an energy-dependent delay effect. A different medium is analogous to a potential barrier. One could imagine an experimental setup in which an incoming photon beam's energy is varied, looking for a characteristic delay dependent on index of refraction for a material. Similar photonic tunneling time experiments have already been carried out[2], but have not examined the threshold energy case.

These results should also be applicable to nuclear fragmentations and collisions. Nuclear potentials have a clearly defined maximum, which nuclear particles must overcome to interact. It might be the case that particles very close to this energy would spend more time interacting, thus slowing down that nuclear process. This experiment would most likely be more difficult to set up, and would probably not be an ideal way to practically study this effect.

3 Methods and Results

3.1 The Step Potential

Using classical mechanics, calculating the reflection time of a particle of mass m incident on a higher-energy step potential is quite simple. The particle's energy is simply $E = \frac{1}{2}mv_0^2$, which can be rewritten $v_0 = \sqrt{\frac{2E}{m}}$. The reflection can be treated as a simple elastic collision, with the particle travelling a distance d to the potential and a distance d back with the same absolute velocity. So $2d = v_0\tau$ and

$$\tau_{c,step} = \sqrt{\frac{2m}{E}}d \tag{1}$$

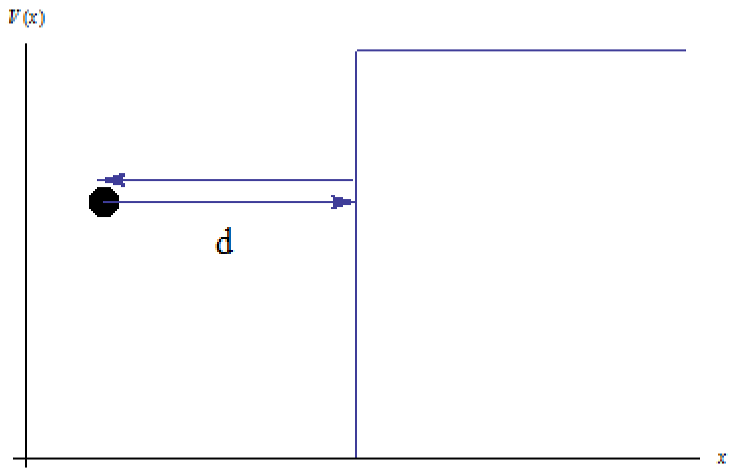

Figure 2: A step potential with an incident classical particle

Finding the Wigner time for a potential is more difficult. The Wigner time is the time it takes for the centroid of a Gaussian wave packet to return to its original position. To find it, we must first find the scattering states by solving the Schrödinger equation, then construct a Gaussian wavepacket out of them. Since they have well-defined time-dependent behavior, so will the Gaussian. For the step potential and $x < 0$, these scattering states are

$$\psi_{sc} = \frac{1}{\sqrt{2\pi}} e^{ipx} + \frac{1}{\sqrt{2\pi}} e^{-ipx} e^{-i\delta(p)} \tag{2}$$

Where δ is a phase shift and p is the momentum. The incoming particle can be represented by a moving Gaussian wavepacket of width σ and wave number k:

$$\psi(x) = Ae^{-\frac{x^2}{2\sigma}} e^{ikx} \tag{3}$$

The momentum-space wavefunction will be the overlap of this with the scattering states:

$$\psi(p) = \int_{-\infty}^{\infty} \psi_{sc}^{*} \psi(x)\, \mathrm{d}x = \sigma A e^{-\frac{\sigma^2}{2}(p-k)^2} \tag{4}$$

Overlapping this with the scattering states, with added time dependence, gives the time-dependent wavefunction:

$$\psi(x,t) = \int_{0}^{\infty} \psi(p) \psi_{sc} e^{-i\frac{\hbar^2 p^2}{2m} t}\, \mathrm{d}p \tag{5}$$

Solving for the difference in time between two instances of the wavepacket being at the starting point gives the Wigner time. The solution has a form proportional to the derivative of the phase shift with respect to the wave number, and is

$$\tau_q = -\frac{m}{k} \frac{\mathrm{d}\delta}{\mathrm{d}k} \tag{6}$$

$$\tau_{q,step} = \sqrt{\frac{2m}{E}} d + \frac{\hbar}{\sqrt{E(V_0 - E)}} \tag{7}$$

The quantum time delay is the classical delay time plus a quantum correction. As V_0 approaches infinity, this agrees with the classical time calculation. This makes sense, since for a larger barrier less and less of the wavefunction becomes a decaying exponential under it. As E approaches V_0, the quantum correction becomes asymptotically large and thus the reflection time becomes large. This is exactly the sort of behavior we are looking for, and this result is therefore quite encouraging.

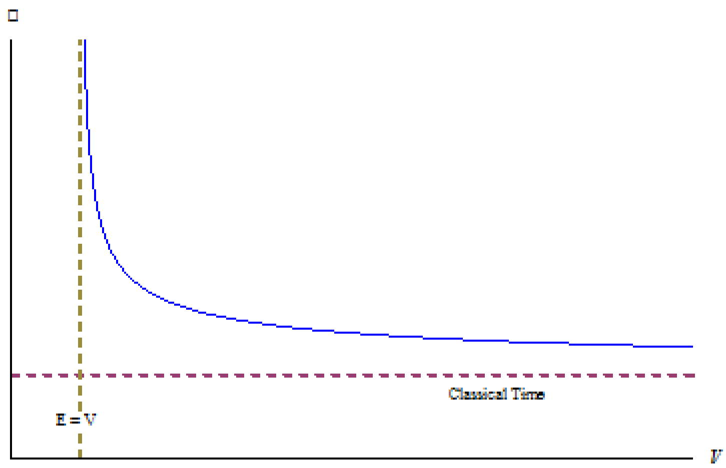

Figure 3: The quantum-corrected reflection time for a step potential

3.2 The Hyperbolic Tangent Potential

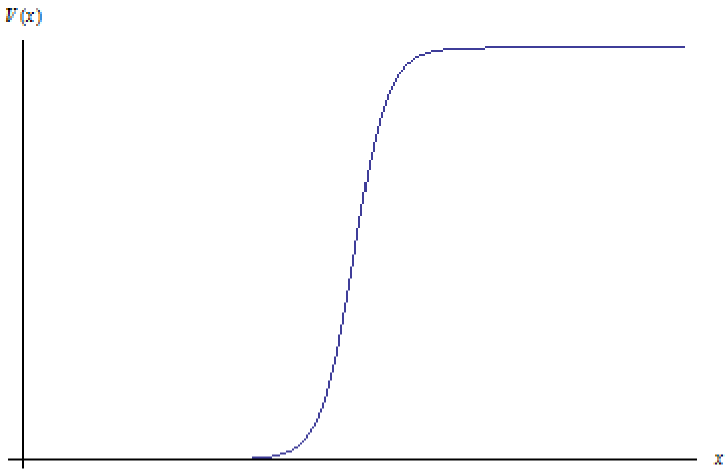

Figure 4: A tanh potential

The potentials for which we've seen near-threshold time delay so far - Schwartz's square potential and the step potential - have had something in common. They both have discontinuous derivatives, and we wanted to determine whether the time delay effect was dependent on this fact. Therefore, our next goal was to solve for a tanh potential, which behaves like a smooth step: It approaches one value at $-\infty$, and another at ∞, but does not change abruptly.

3.2.1 Classical Return Time

We began by solving for the classical time delay using conservation of energy. Since the tanh function approaches, but never quite reaches, the peak energy, we actually expected the classical result to diverge near threshold. For the tanh analysis, we typically used the natural unit system in which $V_0 = \hbar =$

$m = 1$. Our conservation of energy equation was

$$E = \frac{1}{2}v^2(x) + \frac{1}{2}[1 + \tanh(\frac{x}{l})] \tag{8}$$

Which we can solve to obtain $v(x)$. Instead of a simple fraction like the step potential, since the tanh potential varies over x, we need to instead use an integral to find the return time.

$$\tau = 2\int_{-d}^{x_f} \frac{\mathrm{d}x}{v(x)} = 2\int_{-d}^{x_f} \frac{\mathrm{d}x}{\sqrt{2E - 1 - \tanh(\frac{x}{l})}} \tag{9}$$

When solved, this yields

$$\tau = l\sqrt{\frac{2}{1-E}}\tan^{-1}(\sqrt{\frac{E - \frac{1}{2}[1 + \tanh(\frac{x}{l})]}{1-E}}) + l\sqrt{\frac{2}{E}}\tanh^{-1}(\sqrt{\frac{E - \frac{1}{2}[1 + \tanh(\frac{x}{l})]}{E}})|_{-d}^{x_f} \tag{10}$$

At threshold, $x_f = \infty$ and thus $E - \frac{1}{2}[1 + \tanh(\frac{x_f}{l})] = 0$, so the upper limit of integration is 0. Assuming $\frac{d}{l}$ is large, meaning the incoming particle starts at a region of low potential, we can use

$$\tanh(x) \approx 1 - 2e^{-2x},\ \tanh^{-1}(1 - \delta) \approx \frac{1}{2}\log(\frac{2}{\delta}) \tag{11}$$

And the $\tan^{-1}$ term becomes $\frac{\pi}{2}$. Applying these approximations, the classical return time becomes

$$\tau_{c,tanh} = \sqrt{\frac{2}{E}}d + \frac{l}{\sqrt{2}}[\log(4E) + \frac{\pi}{\sqrt{1-E}}] \tag{12}$$

3.2.2 Quantum Return Time: Small *l*

The quantum return time for the tanh potential is obtained in much the same way as for the step, but due to the nature of the potential it was significantly more difficult to solve for. We start with the Schrödinger equation in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{\lambda}{2}[\tanh(\frac{x}{l})+1]\psi=E\psi \tag{13}$$

Choosing to use the natural unit system and simplifying:

$$\frac{1}{2}[\tanh(\frac{x}{l})+1]=\frac{\exp(\frac{2x}{l})}{\exp(\frac{2x}{l})+1} \tag{14}$$

Setting $y=\exp(\frac{2x}{l})$, the Schrödinger equation becomes

$$y^2\frac{d^2\psi}{dy^2}+y\frac{d\psi}{dy}+\frac{l^2}{2}[E-\frac{y}{y+1}]\psi=0 \tag{15}$$

Doing another replacement: $z=\frac{1}{y+1}\to y=\frac{1}{z}-1$

$$\frac{d^2\psi}{dz^2}+[\frac{1-2z}{z(1-z)}]\frac{d\psi}{dz}+\frac{l^2}{2}[\frac{E-(1-z)}{z^2(1-z)^2}]\psi=0 \tag{16}$$

Trying to reach hypergeometric form, substituting $\psi=z^\alpha(1-z)^\beta\phi$:

$$\frac{d\psi}{dz}=z^\alpha(1-z)^\beta\{\frac{\alpha}{z}-\frac{\beta}{1-z}\}\phi \tag{17}$$

$$\frac{d^2\psi}{dz^2}=z^\alpha(1-z)^\beta\{\frac{d^2\phi}{dz^2}+2(\frac{\alpha}{z}-\frac{\beta}{1-z})\frac{d\phi}{dz}+(\frac{\alpha(\alpha-1)}{z^2}-\frac{2\alpha\beta}{z(1-z)}+\frac{\beta(\beta-1)}{(1-z)^2})\phi\}$$

Want to pick α and β such that the $\frac{1}{z^2}$ and $\frac{1}{(1-z)^2}$ terms vanish, since the form of the hypergeometric equation we want does not include them. This yields

$$\frac{l^2E}{2} - \frac{l^2}{2} + \alpha^2 = 0 \rightarrow \alpha = \pm l\sqrt{\frac{1-E}{2}} \tag{18}$$

$$\frac{l^2E}{2} + \beta^2 = 0 \rightarrow \beta = \pm il\sqrt{\frac{E}{2}}$$

Choosing $\alpha = l\sqrt{\frac{1-E}{2}}$ and $\beta = il\sqrt{\frac{E}{2}}$, the differential equation reaches hypergeometric form, which has the solution

$$\phi(z) = {}_2F_1((\alpha+\beta), 1+(\alpha+\beta); 1+2\alpha; z) + z^{-2\alpha}\, {}_2F_1(-(\alpha+\beta), 1-(\alpha+\beta); 1-2\alpha; z) \tag{19}$$

Where ${}_2F_1$ is an ordinary hypergeometric equation. Substituting back in for ψ and x gives the scattering states:

$$\psi_{sc} = \frac{\Gamma(1+2\alpha)\Gamma(2\beta)}{\Gamma(\alpha+\beta)\Gamma(1+\alpha+\beta)} e^{-i(x-d)\sqrt{2E}} + \frac{\Gamma(1+2\alpha)\Gamma(-2\beta)}{\Gamma(\alpha-\beta)\Gamma(1+\alpha-\beta)} e^{i(x-d)\sqrt{2E}} \tag{20}$$

The $(x-d)$ terms are due to the fact that calculations until now have assumed a tanh potential centered around 0, when it should in fact be centered around d. This means that the reflection coefficient is, after some simplification,

$$r = \frac{(\alpha-\beta)\Gamma(2\beta)\Gamma^2(\alpha-\beta)}{(\alpha+\beta)\Gamma(-2\beta)\Gamma^2(\alpha+\beta)} e^{-i2d\sqrt{2E}} = e^{-i\delta} \tag{21}$$

All of the math from the derivation of the Wigner time for the step potential still applies. In natural units, and changing the derivative to something more usable,

$$\tau_q = -\frac{m}{k}\frac{d\delta}{dk} = -\frac{d\delta}{dE} \tag{22}$$

Now, we choose to assume a narrow tanh potential. This means that l, and thus both α and β, are small and we can use a small argument approximation for the Γ functions. For $x << 1$, $\Gamma(x) \approx \frac{1}{x}$, so

$$r \approx -\frac{\alpha+\beta}{\alpha-\beta} e^{-i2d\sqrt{2E}} = e^{-i\delta} \tag{23}$$

$$\tau_{q,small\ l} = \sqrt{\frac{2}{E}} d + \frac{1}{\sqrt{E(1-E))}} \tag{24}$$

3.2.3 Large l

We also wanted to see how the return time would behave for a very wide potential, so we also did this calculation for large l. This makes β large and α arbitrary, rather than both being small as for small l. Under these conditions, $\Gamma(x) \approx \sqrt{2\pi} e^{-x} x^{x-1/2}$. Since there is no transmission, the reflection coefficient will have real magnitude 1, and can be reduced to only a phase. In this regime, it becomes

$$r = e^{i4|\beta|\log(2)} e^{i\frac{\pi}{2}} e^{-i2\pi\alpha} e^{-i2d\sqrt{2E}} \tag{25}$$

$$\rightarrow \delta(E) = \frac{\pi}{2} + 2d\sqrt{2E} + 2\pi\alpha - 4|\beta|\log(2)$$

$$\tau_{q,large\ l} = \sqrt{\frac{2}{E}} d - \frac{l}{\sqrt{2}} [\frac{\log(4)}{\sqrt{E}} + \frac{\pi}{\sqrt{1-E}}] \tag{26}$$

(The minus sign is probably a calculation error, as it doesn't make physical sense and is inconsistent with other calculations. I'll assume in analysis that it should be positive)

3.3 Discussion

Our results for the return time all share some intriguing common features. Without fail, they include the classical return time for a step potential: $\sqrt{\frac{2}{E}}d$. This acts as a consistent baseline time. When we take into account quantum corrections for the step(7), an extra correction is introduced of $\frac{\hbar}{\sqrt{E(V_0-E)}}$. Since E is approaching 1, the first E in the denominator becomes irrelevant. In natural units, therefore, the step correction becomes $\frac{1}{\sqrt{1-E}}$. The quantum correction for a narrow tanh potential(24) gives the exact same return time, as it should: A tanh potential becomes a step potential in the limit $l \to 0$.

More interestingly, this same factor of $\frac{1}{\sqrt{1-E}}$ also appears in the classical derivation of the tanh potential return time(12). We had known that the classical time would diverge, but this result means that it diverges at the same rate as our quantum delay effect. Further, the large l time(26) becomes identically equal to the classical time as it approaches threshold. This suggests that a less abrupt change in potential has the effect of 'weakening' quantum corrections. Even so, the time delay effect we have been searching for seems to be retained across all regimes.

4 Next Steps

4.1 Square and sech Potentials

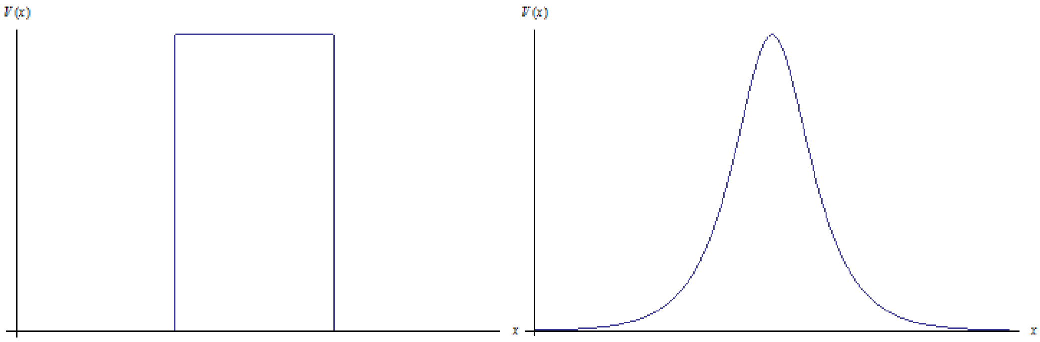

Figure 5: A square and sech potential

Although we have run out of time this year, our goal is a publication, and to that end we still have a few more steps to accomplish. Primarily, we want to see if potentials with a possibility of transmission exhibit the same delay effect. The first step would be to analyze the one Schwartz used, a square potential, analytically rather than numerically. This should not be overly difficult, as the solution for its scattering states is very well understood, and the classical return time would be the same as for a step. The sech potential is to the square as the tanh is to the tanh: It is the smooth analogue. It will most likely be significantly more difficult to analyze, on par with the tanh potential.

4.2 The General Potential

We have the tools at our disposal to approximately solve for any smooth potential, in the form of the WKB Approximation. We have done much of

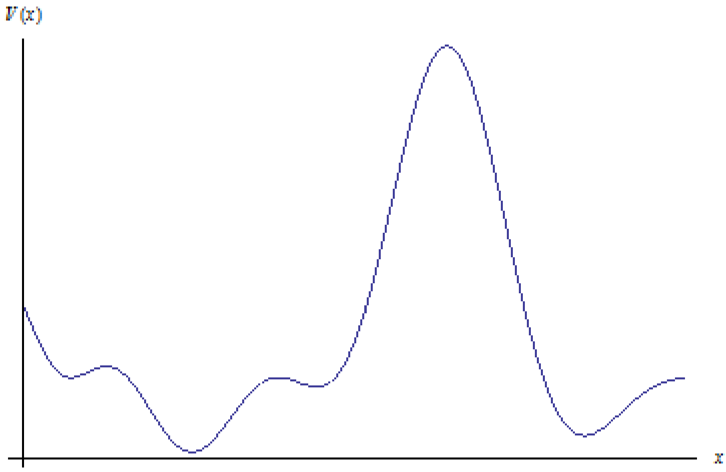

Figure 6: An arbitrary smooth potential

the preliminary analysis, but have not yet found a return time. By assuming a negligable second derivative, WKB gives a solution of the form

$$\psi(x) \approx \frac{C}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x)\,\mathrm{d}x}, \; p(x) \equiv \sqrt{2m(E - V(x))} \tag{27}$$

In textbook WKB, there are regions for which this solution does not apply when the energy crosses the potential and $p(x) \to 0$. In those regions, the procedure is to approximate the potential as linear and solve to produce "joining formulae" in the form of Airy functions. However, this does not apply to our case. We are dealing with near-threshold energies, so the first term of the Taylor expansion would be zero rather than linear. Therefore we instead approximated a negative quadratic potential, $V(x) = -\frac{1}{2}m\omega x^2$. Solving the Schrödinger equation for this potential yields a solution of the form

$$\psi(x) = Ae^{-\frac{i}{4}\beta^2 x^2}\, {}_1F_1(1 + i\frac{E}{2\hbar\omega}, \frac{1}{2}, \frac{i}{2}\beta^2 x^2) \tag{28}$$

This is a confluent hypergeometric function, and it agrees with the WKB solution as $x \to \pm\infty$.

We want to complete analysis of the general potential before publication. This will involve determining the extent of the region over which the WKB solution does not apply, then matching that solution to the joining function. Once we do this we should be able to calculate scattering states, reflection and transmission coefficients, and finally the Wigner time, as with the step and tanh. If it diverges, it will show a greater generality to the delay effect.

4.3 Other Things

Since we will be working with potentials that have transmission as well as reflecion, it could help our analysis to examine energies approaching threshold from greater than V_0 rather than only less. This would allow us to determine what sort of asymptote the threshold energy is, and could grant additional insight into the exact nature of the time delay. While using these energies slightly greater than V_0, we would be interested in transmission time rather than reflection.

We also might look into and try to calculate alternative methods of return time calculation, especially ones proposed by Landauer.[3] He claims that the peak of a Gaussian has no concrete physical meaning, and proposes several alternatives. One of them, involving varying the top of a potential in a time-dependent way, has a listed solution for a square potential which diverges at the threshold.

5 Conclusion

Our hypothesis that near-threshold tunneling is associated with a time delay is looking strong. We first analytically identified this effect, which Schwartz noticed in his numerical calculations, in the quantum return time for a step potential. We found that it persisted in all regimes of a tanh potential, including in classical and both narrow and wide quantum times. While we still have things left to test, Schwartz's original observations, the basis of this project, present evidence that this effect should manifest in systems with allowable transmission as well. It remains to be seen whether it also applies to transmission time, or whether the effect remains for other methods of measuring time, but we will try to figure this out in the near future. There could be many important applications to this research, and I hope it proves useful.

6 Acknowledgements

I would like to thank Professor Tim Atherton for bringing Judah Schwartz's research to our attention, and especially Professor Harsh Mathur for working tirelessly with me on this project.

References

[1] Abraham Goldberg and Harry M. Schey and Judah L. Schwartz, *Computer-Generated Motion Pictures of One-Dimensional Quantum-Mechanical Transmission and Reflection Phenomena*. American Journal of Physics, Volume 35, Number 3, March 1967.

[2] M. Deustch and J.E. Golub, *Optical Larmor clock: Measurement of the photonic tunneling time*. Physical Review A 53, 434, 1996.

[3] R. Landauer and Th. Martin, *Barrier Interaction Time in Tunneling.* RMP Colloquia, January 1992.