1. Setup
    a. The updating scheme in Eq. (2) is clearly unitary. A unitary matrix has Conjugate(U)*U = I. For equation two, each element on the diagonal is $\frac{1 - i\,H\,\Delta t/2}{1 + i\,H\,\Delta t/2} \cdot \frac{1 + i\,H\,\Delta t/2}{1 - i\,H\,\Delta t/2} = 1$ so the matrix is I, and Eq. (2) is unitary.
    b. For dimensionless quantities, we can set $m \approx h = 1$. We want $\varepsilon \ll 1$, so we will use a range of values around 0.01. Likewise, Δt will be 0.01 to 0.001, depending on what we think are acceptable integration step errors.
    c. All code used for this project is found in final_project.py. The analysis and plotting was done using the functions defined in that file in the ipython environment.
2. Wavepacket
    a. For a large k, the packet clearly behaves in the expected manner. A gaussian wavepacket was created with epsilon = 0.005, k = 30, x0 = -0.5, and sigma = 0.25. The magnitude, real, and imaginary parts of this wavefunction are plotting in phi_initial.png. The wavepacket was evolved for 30 steps with delta_t = 0.001. The result is plotted in phi_final.png. The wavepacket is still clearly gaussian and has moved to the right, as we would expect. However, the peak is not as high. This is probably due to edge effects, but it could be the effect of dispersion as well (see the next part). Time evolving this state 30 steps backwards with delta_t = -0.001 gives us the result plotted in phi_back_to_initial.png. We can easily find the mean difference and standard deviation of the initial phi and the rewinded phi. It turns out this is on the order of 10^{-14}, which suggests that the difference is due to numerical precision.
    b. An interesting phenomena is observed at lower energies. For small k, a much larger amount of dispersion is observed that high k. phi0.png contains the plots of the initial wavefunction's magnitude, real, and imaginary parts respectively. This wavepacket had epsilon = 0.001, k = 10, x0 = 0, and sigma = 0.1. phi1.png contains the result of time evolving phi0. The state was evolved 20 times with delta_t of 0.001. It is clear that the state has retained a gaussian form, but has

dispersed, since the packet has become wider and lower. This is partially due to the finite space of the simulation - the edges are affected the wavefunction. However, a gaussian wave packet with zero momentum in a region of V = 0 will disperse, so it is unsurprising we see dispersion in the dynamic case as well, and that it is especially noticeable at low k. However, the process is still consistent with time reversal. phi2.png contains the plots for the phi1 wavefunction evolved 20 steps with delta_t of -0.001. It is clear that the original wavefunction is mostly recovered. In fact, the difference is roughly the same as that found in part a.

3. Step function potential
    a. For the low energy test, an initial wavefunction with epsilon = 0.005, k=1, x0 = -0.3, and sigma = 0.1 was used. This was sent to two step functions, one with a height of 100 and one with a height of 10, both with the step occuring at x = 0. The three plots of the wavefunction can be found in step_function_v10_initial.png, step_function_v10.png, and step_function_v100.png.
    b. We can see in step_function_v100.png that the wavefunction does not make it past the potential barrier. Instead it bounces, and there is a exponential decay in the region x > 0.
    c. For the v = 10 step function (in step_function_v10.png),, we see that some of the wave function is transmitted. The dispersion of the wave function makes it a bit tricky to see, but we can judge based on the packet nearest x = -1 and the packet near to x = 1 that the transmission to reflection ratio is about 1:4.
    d. It would be nice to see these phenomenon without so much dispersion, so it is worth seeing what happens with high k. As a second test wavepacket, we choose a gaussian with epsilon = 0.005, k = 10, x0 = -0.3, and sigma = 0.25. We evolve this wavefunction for 30, 50, and 70 steps of delta_t of 0.001 and set the height of the step function to 25. We observe the wavepacket “bunching up” near the edge of the potential at n = 30, and the wavefunction pass the boundary at n = 50 and n

= 70. The plots that show this evolution are step_function_v25_n(initial, 30,50,70).png.

e. Finally, we send the same wavepacket at a step function with h = 100. The results are found in step_function_v100_n(30,50,70,90).png. Clearly, the wavepacket does not pass the potential and bounces back to the left after compressing to the left of x = 0.

4. Decay of an unstable state

a. For the first test, I used a width of 0.5 and epsilon of 0.001. This state is plotted in unstable_state_initial.png. I evolved this state 15 steps of delta_t = 0.001. This wavefunction is plotted in unstable_state_n15.png. The result makes sense - we see some tunneling, but most of the wavefunction remains in the pocket of the initial wavefunction. The oscillations in the real and imaginary part of the wavefunction could be interpreted as oscillations heading off to infinity. The state was evolved for 15 more steps and the resulting wave function is plotted in unstable_state_n30.png. This wavefunction shows definite oscillatory behavior outside the pocket. The wavefunction has also "clumped" around the edges of the pocket. This is similar to the behavior of a wavepacket in a simple harmonic oscillator, and probably indicates the energy of the resonant state is higher than the boundaries of the pocket.

b. The solution to the resonant state having higher energy than the pocket is to simply raise the walls. The initial unstable state was kept the same, as were the dimensions of the pocket, but the walls were raised to h = 100. These results represent the decay much better. The time evolution of the state can be found in h100_unstable_state_n(15,30,45).png. The plots clearly show the probability density leaking out of the pocket as well as oscillatory behavior outside the pocket.

c. From the better results in part b, we can estimate the decay rate. To do this we can simply integrate phi*phi inside the pocket and compare it to the integral of phi*phi outside the pocket. Since we are working in discrete space, this is just a

sum. The probability the particle is inside the pocket versus time is plotted in prob_inside_pocket.png. The graph is generally exponential, which is what we would expect. It seems to take some time to reach exponential decay, and at the end, it becomes noisy, which must be a result of the boundaries and the particle bouncing back into the pocket. However, we can estimate the decay rate from the middle section of the data. Doing some basic calculations, we find the decay rate to be abou 26.0 s^{-1}. It should be noted that the exponential fit is not a very good one, however. To get more reliable results a smaller delta_t should be used, to get good results in the phase that seems like exponential decay.

5. Scattering
    a. For scattering off the pocket potential, the gaussian wavepacket that gave the clearest results and the potential that gave the clearest results were chosen. The wavepacket is a gaussian with epsilon = 0.005, k = 10, x0 = -0.5, and sigma = 0.25, while the pocket potential has a width = 0.25, s = 0.1, b = 0.5, and h = 100. The results of this scattering are plotted in pocket_scattering_(initial, n15, n30, n45, n60).png for 0, 15, 30, 45, and 60 iterations of delta_t = 0.001 respectively. We observe what we would qualitatively expect. The wavepacket hits the first barrier, and some probability leaks through into the center of the pocket. Over time, the probability of finding the particle in the pocket grows and moves left. It hits the second barrier in the pocket potential and “bunches up” there, but some probability leaks through and displays oscillatory behavior like the sine packet in part 4. This is encouraging and suggests that a gaussian wavepacket with k = 10 has a similar energy to the sine wavefunction in part 4. In the final state, we see roughly the same probability of finding the particle in the pocket and to the left of the pocket.
    b. When we lower the energy of the incident wavepacket, we would expect the wavepacket to be reflect from the pocket potential with very little tunneling. This is what we in fact observe. Using the same wavepacket as part a, but with k = 1

rather than 10, we see the wavepacket bounce back from the first barrier. This evolution is shown in low_e_pocket_scattering_(n15, n30, n45, n60).png.

c. For high energy we would expect the wavepacket to make it through the pocket potential with little or no change. When we really increase the gaussian energy to high levels (k above 100), we see this exactly. This is not terribly interesting to plot, so I reduced the gaussian wavepacket k to 30. The results are plotted in high_e_pocket_scattering_(n10, n20, n30, n40).png. It is clear that at this energy, the wavepacket is affected by the pocket potential. At n10 and n30 we see the particle stall near the barriers. However, by n40, the particle has moved completely past the potential (and is hitting the ill-defined boundary conditions).