PHY407 Lab 9: Partial Differential Equations, Pt. II

Work Distribution:
Emma Jarvis: Q1, Q3
Lisa Nasu-Yu: Q2

November 19, 2021

1 Solving the Wave Equation with the Spectral Method

1.a

To show that 2 solves 1, we need to take the second order t and x derivatives of 2 and sub these into 2, and also check the boundary and initial conditions 3, 4 and 5 to ensure the equation is solved.

$$\frac{\partial^2 \phi}{\partial t^2} = \nu^2 \frac{\partial^2 \phi}{\partial x^2} \tag{1}$$

$$\phi(x,t) = \sum_{k=1}^{\infty} \sin\frac{k\pi x}{L}\left[\tilde{\phi}_{0,k}\cos\omega_k t + \frac{\tilde{\psi}_{0,k}}{\omega_k}\sin\omega_k t\right] \tag{2}$$

$$\phi(x=0) = \phi(x=L) = 0 \tag{3}$$

$$\phi(t=0) = \phi_0 = \sum_{k=1}^{\infty} \tilde{\phi}_{0,k}\sin\frac{k\pi x}{L} \tag{4}$$

$$\psi(t=0) = \psi_0 = \frac{\partial \phi}{\partial t}(t=0) = \sum_{k=1}^{\infty} \tilde{\psi}_{0,k}\sin\frac{k\pi x}{L} \tag{5}$$

These derivatives of 2 are given by 6 and 7.

$$\frac{\partial^2 \phi}{\partial t^2} = \sum_{k=1}^{\infty} \sin\frac{k\pi x}{L}\left[-\omega_k^2\tilde{\phi}_{0,k}\cos\omega_k t - \frac{\tilde{\psi}_{0,k}}{\omega_k}\omega_k^2\sin\omega_k t\right] \tag{6}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \sum_{k=1}^{\infty} -\frac{k^2\pi^2}{L^2}\sin\frac{k\pi x}{L}\left[\tilde{\phi}_{0,k}\cos\omega_k t + \frac{\tilde{\psi}_{0,k}}{\omega_k}\sin\omega_k t\right] \tag{7}$$

Setting 6 = 7 we can see that

$$\frac{k\pi}{L} = \omega_k$$

. This solution also satisfies the boundary conditions, 3 by setting $x = 0$ the equation becomes

$$\phi(0,t) = \sum_{k=1}^{\infty} \sin\frac{k\pi 0}{L}\left[\tilde{\phi}_{0,k}\cos\omega_k t + \frac{\tilde{\psi}_{0,k}}{\omega_k}\sin\omega_k t\right] = \sum_{k=1}^{\infty} \sin 0\left[\tilde{\phi}_{0,k}\cos\omega_k t + \frac{\tilde{\psi}_{0,k}}{\omega_k}\sin\omega_k t\right] = 0$$

and setting $x = L$

$$\phi(L,t) = \sum_{k=1}^{\infty} \sin \frac{k\pi L}{L} \left[\tilde{\phi}_{0,k} \cos \omega_k t + \frac{\tilde{\psi}_{0,k}}{\omega_k} \sin \omega_k t \right] = \sum_{k=1}^{\infty} \sin k\pi \left[\tilde{\phi}_{0,k} \cos \omega_k t + \frac{\tilde{\psi}_{0,k}}{\omega_k} \sin \omega_k t \right] = 0$$

It also satisfies the initial conditions 4 and 5 by setting $t = 0$, 2 becomes

$$\phi(x,0) = \sum_{k=1}^{\infty} \sin \frac{k\pi x}{L} \left[\tilde{\phi}_{0,k} \cos \omega_k 0 + \frac{\tilde{\psi}_{0,k}}{\omega_k} \sin \omega_k 0 \right] = \phi(x,t) = \sum_{k=1}^{\infty} \sin \frac{k\pi x}{L} \tilde{\phi}_{0,k} = \phi_0$$

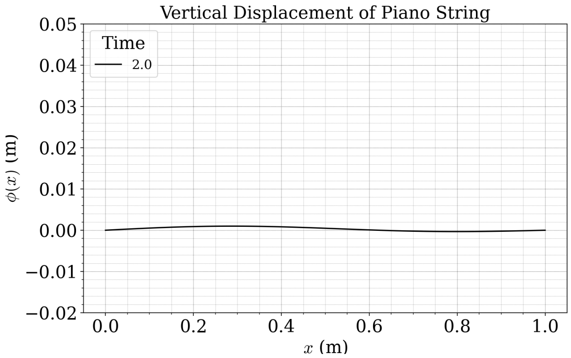
and

$$\frac{\partial \phi}{\partial t}(t=0) = \sum_{k=1}^{\infty} \sin \frac{k\pi x}{L} \left[-\omega_k 0 \tilde{\phi}_{0,k} \sin \omega_k 0 + \frac{\omega_k 0 \tilde{\psi}_{0,k}}{\omega_k} \cos \omega_k 0 \right] = \sum_{k=1}^{\infty} \sin \frac{k\pi x}{L} \tilde{\psi}_{0,k} = \psi_0$$

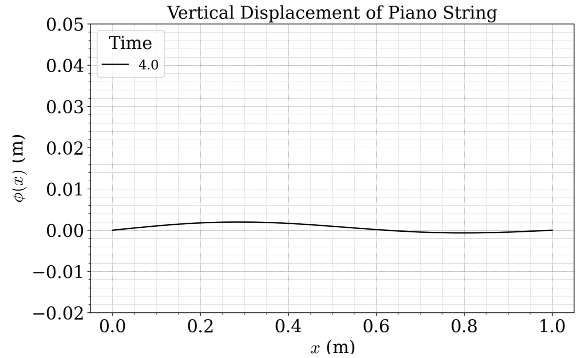
.

1.b

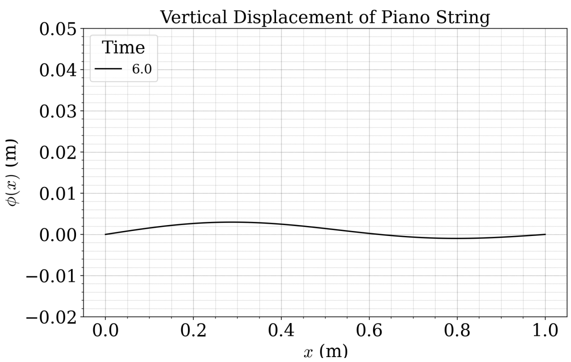
We then used a series solution to plot $\phi(x,t)$ for times of 2, 4 6, 12 100ms. These solutions are depcited in figures 1a, 1b, 1c, 1d and 1e.



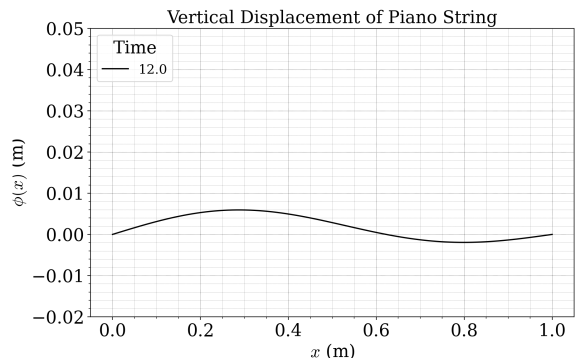
(a) t = 2 ms



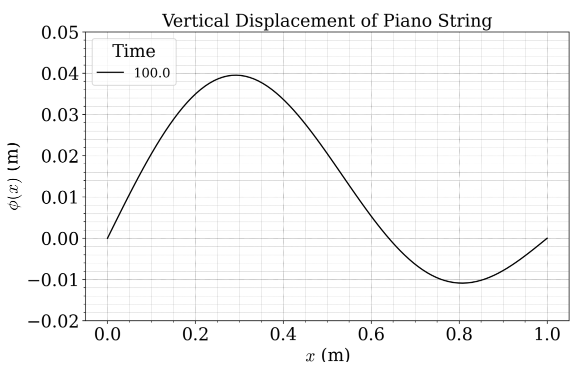
(b) t = 4 ms



(c) t = 6 ms



(d) t = 12 ms



(e) t = 100 ms

Figure 1: The solution to 2 at times 2ms, 4ms, 6ms, 12 ms and 100ms, using the spectral method.

1.c

The spectral method uses Fourier transforms whereas the FTCS is a finite difference method. Compared to the FTCS solution, the spectral method solution does not become unstable after 100ms. Also, using the spectral method, we do not have to step into each time step to evaluate the solution but we can just evaluate the solution at specific values of t. However, the boundary condition has to be simple for the spectral method whereas FTCS can handle more complicated boundaries. Both methods take approximately the same time.

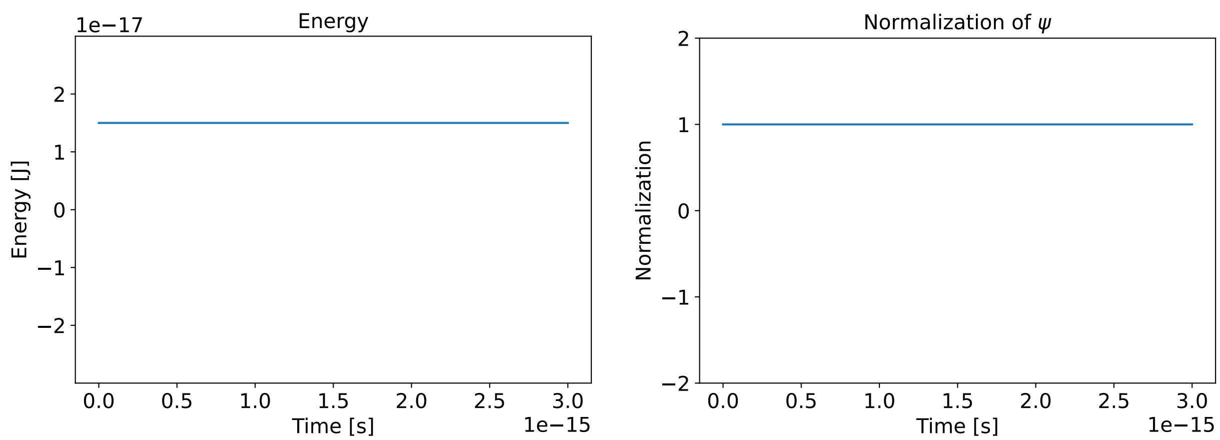
2 Solving the time-dependent Schrödinger equation with the Crank-Nicolson scheme

2.a

We coded the Crank-Nicolson for the time-dependent Schrodinger equation for an infinite square well. The simulation was run for N=3000 time steps, with each time step being $10^{-18}s$.We computed ψ_0 in the initial condition of ψ by requiring ψ to be normalized, such that

$$1 = \int_{\infty}^{\infty} |\psi_0 exp(-\frac{(x-x_0)^2}{4\sigma^2} + i\kappa x)|^2 dx \tag{8}$$

$$\psi_0^2 = \frac{1}{\int_{\infty}^{\infty} |exp(-\frac{(x-x_0)^2}{4\sigma^2} + i\kappa x)|^2 dx} \tag{9}$$



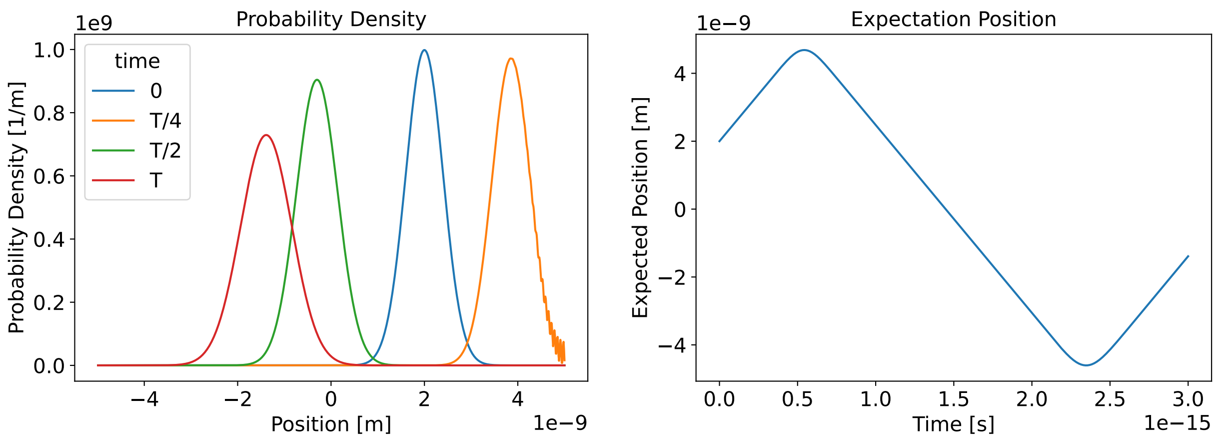
(a) Energy

(b) Normalization

Figure 2: Time evolution of the expectation values for energy (Figure a) and normalization (Figure b) for a wavefunction ψ. The energy is constant and the wavefunction is normalized throughout the entire time evolution, as wanted.

2.b

We plot the probability density of the wavefunction Fig. 3a throughout its time evolution. We see that the peak probability moves to the right, then is reflected back within the potential well boundaries. As the quote about the Ehrenfest theorem states, the expectation value of the position for this wavefunction did follow a classical trajectory, shown in Fig. 3b.



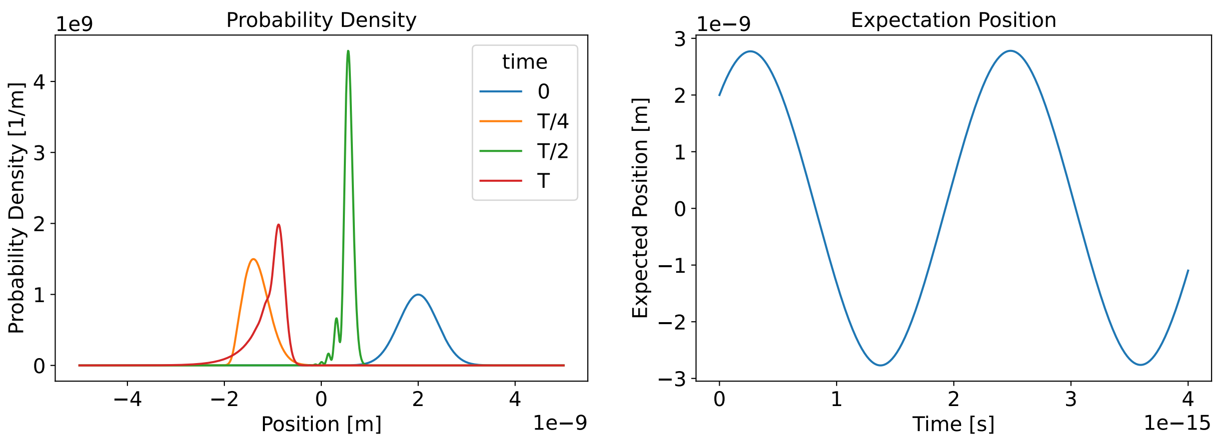
(a) Probability Density

(b) Position

Figure 3: Time evolution of the probability density, $\psi^*\psi$ (Figure a), and expectation values for position (Figure b). The potential was that of an infinite square well.

2.c

We repeated the above for a harmonic potential with $w = 3 \times 10^{15} rads^{-1}$, and a duration of 4000 time steps. Again, we plotted the probability density. The wavefunction oscillates between the boundaries.



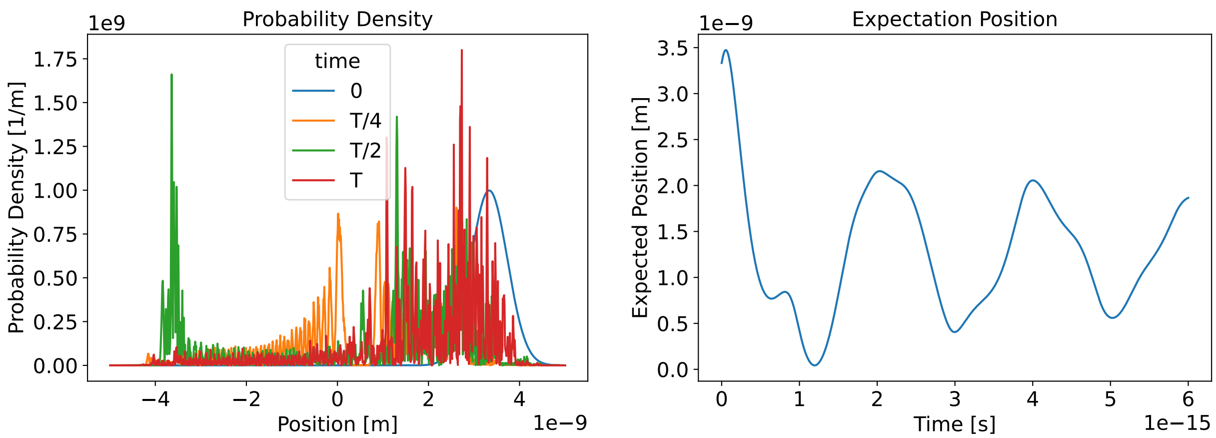
(a) Probability Density

(b) Position

Figure 4: Time evolution of the probability density, $\psi^*\psi$ (Figure a), and expectation values for position (Figure b) for a harmonic potential.

2.d

Finally, we repeated the process for a double well potential.



(a) Probability Density

(b) Position

Figure 5: Time evolution of the probability density, $\psi^*\psi$ (Figure a), and expectation values for position (Figure b) for a double well potential. The probability densities do not have as clear a peak as the previous 2 cases and there is not an obvious pattern to the expectation position.

3 Solving Burger's equation using Lax-Wendroff

3.a

We then derived an expression to solve Burgers' equation using the Lax-Wendroff method. To begin, we used a Taylor expansion to estimate the time derivative as

$$u(x,t+\Delta t) = u(x,t) + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}(\Delta t)^2$$

then using

$$\frac{\partial u}{\partial t} + \epsilon \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = 0 \Rightarrow \frac{\partial u}{\partial t} = -\epsilon \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) \Rightarrow \frac{\partial u}{\partial t} = -\epsilon u \frac{\partial u}{\partial x} \Rightarrow \frac{\partial^2 u}{\partial t^2} = -\epsilon \frac{\partial u}{\partial t}\frac{\partial u}{\partial x}$$

and substituting the expression for $\frac{\partial u}{\partial t}$ gives

$$\frac{\partial^2 u}{\partial t^2} = -\epsilon\left(-\epsilon \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right)\right)\frac{\partial u}{\partial x} \Rightarrow \frac{\partial^2 u}{\partial t^2} = \epsilon^2 \frac{\partial}{\partial x}\left[u \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right)\right]$$

as required. Then substituting this and the above into the equation for $u(x,t+\Delta t)$ gives

$$u(x,t+\Delta t) = u(x,t) - \epsilon \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right)\Delta t + \frac{1}{2}\epsilon^2 \frac{\partial}{\partial x}\left[u \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right)\right](\Delta t)^2$$

as required. Approximating the x-derivatives using central different approximations according to the lab manual gives

$$\frac{\partial u^2}{\partial x} = \frac{(u^j_{i+1})^2 - (u^j_{i-1})^2}{2\Delta x}$$

and

$$\frac{\partial u^2(x \pm \Delta x/2, t)}{\partial x} = \frac{(u^j_{i\pm1})^2 - (u^j_i)^2}{\pm \Delta x}$$

and

$$u(x \pm x/2, t) = \frac{u_i^j + u_{i\pm1}^j}{2}$$

Substituting these into the expression for $u(x, t + \Delta t)$ gives

$$u(x, t + \Delta t) = u_i^{j+1} =$$

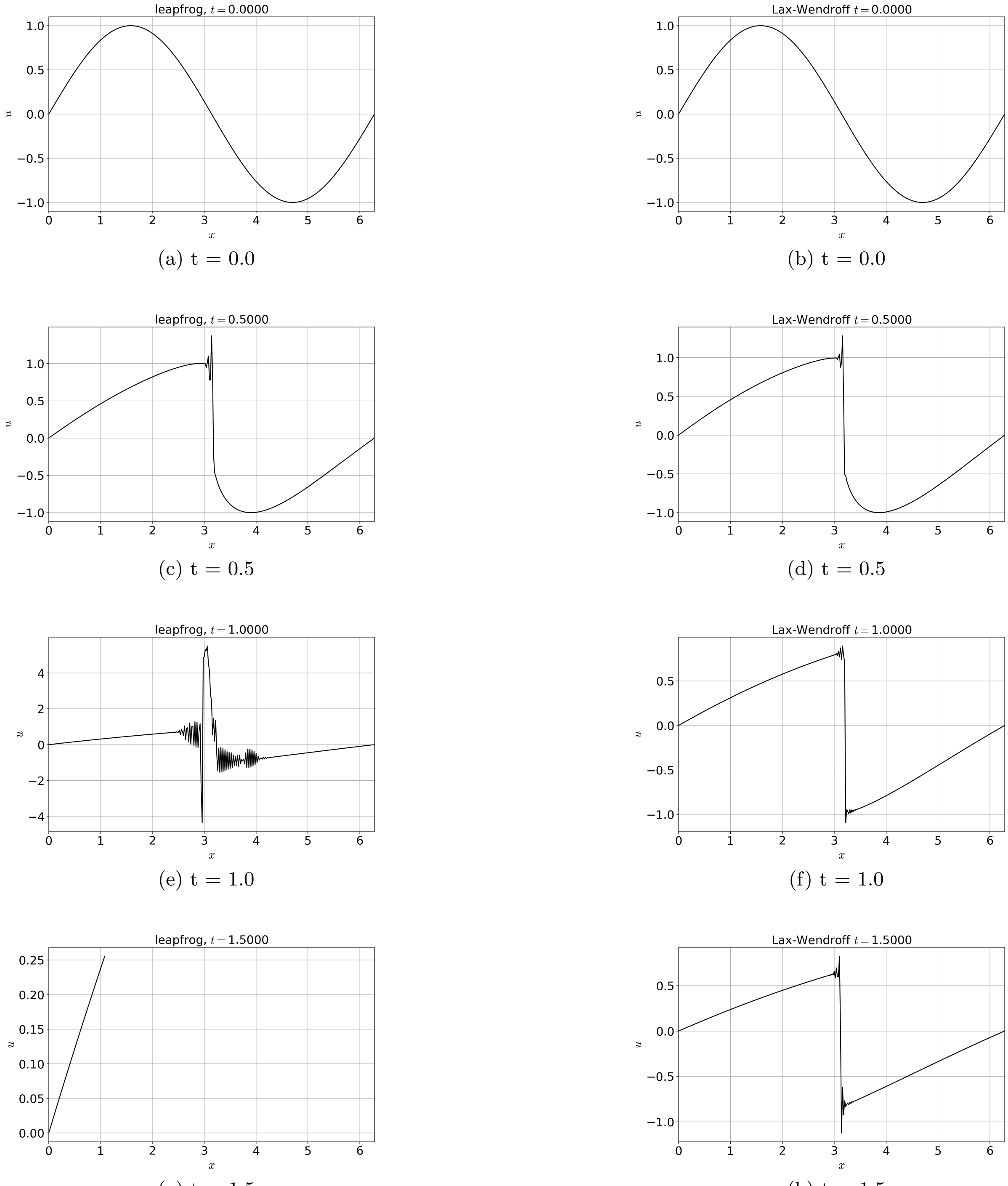
$$u(x,t) - \epsilon \frac{(u_{i+1}^j)^2 - (u_{i-1}^j)^2}{2\Delta x} \Delta t + \frac{1}{2}\epsilon^2 (\Delta t)^2 \frac{1}{\Delta x} \left[\frac{u_i^j + u_{i+1}^j}{2} \frac{(u_{i+1}^j)^2 - (u_i^j)^2}{+\Delta x} - \frac{u_i^j + u_{i-1}^j}{2} \frac{(u_{i-1}^j)^2 - (u_i^j)^2}{-\Delta x} \right]$$

$$= u_i^j - \frac{\beta}{2}(u_{i+1}^j)^2 - (u_{i-1}^j)^2 + \frac{\beta^2}{4} \left[\left(u_i^j + u_{i+1}^j \right) \left((u_{i+1}^j)^2 - (u_i^j)^2 \right) + \left(u_i^j + u_{i-1}^j \right) \left((u_{i-1}^j)^2 - (u_i^j)^2 \right) \right]$$

where $\beta = \frac{\epsilon \Delta t}{\Delta x}$

3.b

We then implemented code to solve Burgers' equation using this equation with the same parameters as Q3 of Lab08 with time steps $t = 0, 0.5, 1, 1.5$ and compared these to the solutions obtained using the leapfrog method in Lab 08. We used the code from the solution of Lab08 and just modified it to include the Lax-Wendroff. Figures 6a, 6c, 6e and 6g depict the leap frog method solution from Lab 08 and figures 6b, 6d, 6f and 6h depict the Lax-Wandroff solutions. The difference is that the leapfrog method fails after 0.5 seconds while the L-W method works pretty well except for the sharp peaks.



(a) t = 0.0

(b) t = 0.0

(c) t = 0.5

(d) t = 0.5

(e) t = 1.0

(f) t = 1.0

(g) t = 1.5

(h) t = 1.5

Figure 6: Solutions to the Burger's equation using leapfrog method for times 0, 0.5, 1.0 and 1.5.