Physics 141 HW 3

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1 Problem 1

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \tag{1}$$

1.1 a

Consider forward Euler for the time discretization. For the approximation of the first order spatial derivative, we consider a scheme known as upwind differencing which uses the value of the solution from the upstream(or "upwind") point. For example, if the wave is moving to the right (c¿0), we use the local value and the value of the neighbor on the left, approximatin the first order spatial derivative as:

$$\frac{\partial u}{\partial t}(x,t) \approx \frac{u(x,t) - u(x-a,t)}{a} \tag{2}$$

Suppose the spatial domain is discretized with uniformly spaced grid points with a grid spacing of a and the time step h, the numerical scheme can be written as:

$$u(x,t+h) = u(x,t) - \frac{ch}{a}(u(x,t) - u(x-a,t)) \tag{3}$$

Use Von Neumann stability analysis to determine the stability conditions for this scheme. Specifically, analyze how a Fourier mode $\delta u(x,t) = \delta\hat{u}(x,t)e^{ikx}$ evolves in time and prove that the stability condition is that the Courant number C satisfies

$$0 \leq C \equiv \frac{ch}{a} \leq 1 \tag{4}$$

1.1.1 Solution

$$u(x,t) = \hat{u}(x,t) + \delta u(x,t) = \hat{u}(x,t) + \delta\hat{u}(x,t)e^{ikx} \tag{5}$$

$$\delta\hat{u}(x,t)e^{ikx} = \sum_k c_k(t)e^{ikx} \tag{6}$$

$$u(x,t) = \hat{u}(x,t) + \delta u(x,t) \tag{7}$$

$\hat{u}$ resistant to small perturbations:

$$u(x,t+h) = u(x,t) - \frac{ch}{a}(u(x,t) - u(x-a,t)) \tag{8}$$

$$= \hat{u}(x,t) + \sum_k c_k(t)e^{ikx} - \frac{ch}{a}(\left(\hat{u}(x,t) + \sum_k c_k(t)e^{ikx}\right) - \left(\hat{u}(x-a,t) + \sum_k c_k(t)e^{ik(x-a)}\right)) \tag{9}$$

$$u(x,t+h) = \hat{u}(x,t) + \sum_k c_k(t)e^{ikx}\left[1 - \frac{ch}{a} + \frac{ch}{a}e^{-ika}\right] \tag{10}$$

$$u(x,t+h) = \hat{u}(x,t+h) + \sum_k c_k(t+h)e^{ikx} \tag{11}$$

$$\hat{u}(x,t+h) + \sum_k c_k(t+h)e^{ikx} = \hat{u}(x,t) + \sum_k c_k(t)e^{ikx}\left[1 - \frac{ch}{a} + \frac{ch}{a}e^{-ika}\right] \tag{12}$$

$$\frac{c_k(t+h)}{c_k(t)} = G = \left[1 - \frac{ch}{a} + \frac{ch}{a}e^{-ika}\right] \tag{13}$$

Note that $|G|^2 \overset{!}{\leq} 1$ in order for the scheme to be stable. Now substitute $C \equiv \frac{ch}{a}$. The worst case(largest) here is when $e^{-ika} = 1$ because we are dealing with real valued a, k.

$$12C + 2C + C^2 2C^2 + C^2 \leq 1 \tag{14}$$

Which admits all possible values for C

The worst case(smallest) is when $e^{-ika} = -1$

$$12C - 2C + C^2 + 2C^2 + C^2 \leq 1 \tag{15}$$

$$1 - 4C - 4C^2 = (1-2C)^2 \leq 1 \tag{16}$$

Which admits solutions:
$0 \leq C \leq 1$.
(Clearly seen from the graph because it is a Parabola with vertex (0.5,0) and points (0,1),(1,1)).

1.2 b

Show that upwinding scheme below effectively introduces a "numerical diffusion" to the equation, which serves to dampen any oscillations in the solution.

$$\frac{\partial u}{\partial t} = -\frac{c}{a}\left(u(x,t) - u(x-a,t)\right) \tag{17}$$

1.2.1 Solution

Taylor expansion of $u(x-a,t)$ around $a=0$ with constant t:

$$u(x-a,t) = u(x,t) - a\frac{\partial u}{\partial x} + a^2\frac{\partial^2 u}{\partial x^2} + \mathcal{O}(a^3) \tag{18}$$

$$\frac{\partial u}{\partial t} = -\frac{c}{a}\left(u(x,t) - u(x,t) + a\frac{\partial u}{\partial x} - a^2\frac{\partial^2 u}{\partial x^2}\right) \tag{19}$$

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = ca\frac{\partial^2 u}{\partial x^2} \tag{20}$$

1.3 b

Show that forward Euler downwind differencing is unstable, that is, that the following scheme is unstable if $c > 0$.

$$u(x,t+h) = u(x,t) - \frac{ch}{a}\left(u(x+a,t) - u(x,t)\right) \tag{21}$$

1.3.1 Solution

From before, we have:

$$u(x,t) = \hat{u}(x,t) + \sum_k c_k(t)e^{ikx} \tag{22}$$

This gives:

$$u(x,t+h) = \hat{u}(x,t) + \sum_k c_k(t)e^{ikx} - \frac{ch}{a}\left(\hat{u}(x,t) + \sum_k c_k(t)e^{ik(x+a)} - \hat{u}(x,t) - \sum_k c_k(t)e^{ikx}\right) \tag{23}$$

$$\hat{u}(x,t+h) + \sum_k c_k(t+h)e^{ikx} = \hat{u}(x,t) + \sum_k c_k(t)e^{ikx} - \frac{ch}{a}\left(\sum_k c_k(t)e^{ik(x+a)} - \sum_k c_k(t)e^{ikx}\right) \tag{24}$$

$$c_k(t+h)e^{ikx} = c_k(t)e^{ikx} - \frac{ch}{a}\left(c_k(t)e^{ik(x+a)} - c_k(t)e^{ikx}\right) \tag{25}$$

$$c_k(t+h) = c_k(t)\left[1 - \frac{ch}{a}\left(e^{ika} - 1\right)\right] \tag{26}$$

$$G = \left[1 - \frac{ch}{a}\left(e^{ika} - 1\right)\right] \tag{27}$$

Taking $C = \frac{ch}{a}$:

$$G = 1 + C - Ce^{ika} \tag{28}$$

$$G^2 = 1 + 2C - 2Ce^{ika} + C^2 - C^2e^{ika} + C^2e^{2ika} \tag{29}$$

Apply same min/max argument to e^{ika}: max: $e^{ika} = -1$

$$G^2_{min} = 1 + 2C - 2C + C^2 - 2C^2 + C^2 = 1 \leq 1 \tag{30}$$

This does not restrict C at all.

min: $e^{ika} = -1$

$$G^2_{min} = 1 + 2C + 2C + C^2 + 2C^2 + C^2 = 1 + 4C + 4C^2 = (2C + 1)^2 \leq 1 \tag{31}$$

Which admits no positive solutions for C. Hence this scheme is unstable

1.4 c

Show that forward Euler central differencing is also unstable, that is, the following scheme is unstable regardless of the sign of c.

$$u(x, t + h) = u(x, t) - \frac{ch}{a}\left(u(x + a, t) - u(x - a, t)\right) \tag{32}$$

1.4.1 Solution

$$u(x, t + h) = u(x, t) - \frac{ch}{a}\left(u(x + a, t) - u(x - a, t)\right) \tag{33}$$

$$c_k(t + h) = c_k(t)\left[1 - C\left(e^{ika} - e^{-ika}\right)\right] = c_k(t)\left[1 - 2iC \sin ka\right] \tag{34}$$

$$G = [1 - 2iC \sin ka] \tag{35}$$

$$G^2 = [1 - 2iC \sin ka] \cdot [1 + 2iC \sin ka] \tag{36}$$

$$G^2 = 1 + 4C^2 \sin ka \tag{37}$$

Apply same min-max:

$$1 + 4C^2(1) \leq 1 \tag{38}$$

$$C^2 \leq 0 \tag{39}$$

Forces c to be imaginary

$$1 + 4C^2(-1) \leq 1 \tag{40}$$

$$C^2 \geq 0 \tag{41}$$

$$\tag{42}$$

c must be real.

Combining these two, it becomes clear that there is no such $c \neq 0$ that makes the scheme stable.

1.5 d

Write down the scheme for **backward** Euler upwind differencing scheme for $c > 0$, and show that it is unconditionally stable.

1.5.1 Solution

Backward Euler upwind differencing scheme must be

$$u(x, t-h) = u(x,t) - \frac{ch}{a}\left(u(x,t) - u(x-a,t)\right) \tag{43}$$

This gives:

$$c_k(t-h) = c_k(t)\left[1 - C + Ce^{ika}\right] \tag{44}$$

$$G = \frac{c_k(t-h)}{c_k(t)} = \left[1 - C + Ce^{ika}\right] \tag{45}$$

$$G^2 = 1 - 2C + 2Ce^{ika} + C^2 - 2C^2e^{ika} + C^2e^{ika} \tag{46}$$

Apply min-max argument:

$$1 - 2C + 2C(1) + C^2 - 2C^2(1) + C^2(1) = 1 \leq 1 \tag{47}$$

Puts no restrictions on C

$$1 - 2C + 2C(-1) + C^2 - 2C^2(-1) + C^2(1) \tag{48}$$

$$= 1 - 4C \leq 1 \tag{49}$$

$$-4C \leq 0 \tag{50}$$

Which just requires that $c > 0$, which is our original domain. Therefore, this scheme is unconditionally stable.

2 Problem 2

In this problem, you will numerically solve the time-dependent Schrödinger equation in one spatial dimension with a step potential. You will investigate how a rightward-moving wave packet interacts with a sudden potential increase and examine its reflection and transmission properties.

Consider the time-dependent Schrödinger equation(in $\hbar = m = 1$ units):

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi \tag{51}$$

on the domain $-L \leq x \leq L$.

The potential is a step function:

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases} \tag{52}$$

Use Dirichlet boundary conditions:

$$\psi(-L,t) = 0; \psi(L,t) = 0 \tag{53}$$

The initial wave packet is a rightward-moving Gaussian:

$$\psi(x,0) = A\exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right)e^{ik_0x}$$

where A is a normalization constant, $x_0 < 0$, σ is the packet width, and $k_0 > 0$ is the central wavenumber leading to a right-moving average momentum.

For clarity, ξ will be used to describe $\frac{\partial\psi}{\partial t}$

2.1 a

From the stability point of view, explain why the Crank-Nicolson method is a good choice for solving the time-dependent Schrödinger equation numerically. Use Von Neumann stability analysis to analyze the growth or decay of the wave function over time.

2.1.1 Explanation

2.1.2 Stability analysis

Decomposition of ψ into Mean Field (hat) portion and Fourier mode perturbations.

$$\psi(x,t) = \hat{\psi}(x,t) + \textstyle\sum_k c_k(t)e^{ikx}.$$

(Note that $\hat{\psi}$ is invariant under small perturbations.)

Using the solution to part b and substituting this identity, we have:

$$\left(\hat{\psi}(x,t+h) + \sum_k c_k(t+h)e^{ikx}\right)\left(1+\frac{h}{2i}V(x)\right) - \frac{h}{2i}\left(\hat{P}(x,t+h) + \sum_k P_k(t+h)e^{ikx}\right) \tag{54}$$

$$= \left(\hat{\psi}(x,t) + \sum_k c_k(t)e^{ikx}\right)\left(1+\frac{h}{2i}V(x)\right) + \frac{h}{2i}\left(\hat{P}(x,t) + \sum_k P_k(t)e^{ikx}\right) \tag{55}$$

With $P_k(t) = c_k(t)\left(e^{ika} + e^{-ika} - 2\right) = c_k(t)\sin^2(\frac{ka}{2})$.

Simplifying,

$$\left(\sum_k c_k(t+h)e^{ikx}\right)\left(1+\frac{h}{2i}V(x)\right) - \frac{h}{2i}\left(\sum_k P_k(t+h)e^{ikx}\right) \tag{56}$$

$$= \left(\sum_k c_k(t)e^{ikx}\right)\left(1+\frac{h}{2i}V(x)\right) + \frac{h}{2i}\left(\sum_k P_k(t)e^{ikx}\right) + \frac{h}{i}\hat{P}(x,t) \tag{57}$$

$$\left(\sum_k c_k(t+h)e^{ikx}\right)\left(1+\frac{h}{2i}V(x) - \frac{h}{2i}\sin^2(\frac{kx}{2})\right) \tag{58}$$

$$= \left(\sum_k c_k(t)e^{ikx}\right)\left(1+\frac{h}{2i}V(x) + \frac{h}{2i}\sin^2(\frac{kx}{2})\right) + \frac{h}{i}\hat{P}(x,t) \tag{59}$$

If we take $\hat{P}(x,t) = 0$, this gives

$$c_k(t+h)\left(1 + \frac{h}{2i}V(x) - \frac{h}{2i}\sin^2(\frac{kx}{2})\right) = c_k(t)\left(1 + \frac{h}{2i}V(x) + \frac{h}{2i}\sin^2(\frac{kx}{2})\right) \tag{60}$$

$$G = \frac{c_k(t+h)}{c_k(t)} = \frac{1 + \frac{h}{2i}V(x) + \frac{h}{2i}\sin^2(\frac{kx}{2})}{1 + \frac{h}{2i}V(x) - \frac{h}{2i}\sin^2(\frac{kx}{2})} = \frac{1 - \frac{ih}{2}V(x) - \frac{ih}{2}\sin^2(\frac{kx}{2})}{1 - \frac{ih}{2}V(x) + \frac{ih}{2}\sin^2(\frac{kx}{2})} \tag{61}$$

Taking the maximal difference ($\sin^2(\frac{kx}{2}) = 1$) between the numerator and denominator gives

$$|G|^2 = GG^* = \frac{1 - \frac{ih}{2}V(x) - \frac{ih}{2}\sin^2(\frac{kx}{2})}{1 - \frac{ih}{2}V(x) + \frac{ih}{2}\sin^2(\frac{kx}{2})} \cdot \frac{1 + \frac{ih}{2}V(x) + \frac{ih}{2}\sin^2(\frac{kx}{2})}{1 + \frac{ih}{2}V(x) - \frac{ih}{2}\sin^2(\frac{kx}{2})} \tag{62}$$

$$= \frac{1 + \frac{h^2}{4}V^2(x) + \frac{h^2}{4}\sin^4(\frac{kx}{2}) + 2\frac{h^2}{4}V(x)\sin^2(\frac{kx}{2})}{1 + \frac{h^2}{4}V^2(x) + \frac{h^2}{4}\sin^4(\frac{kx}{2}) - 2\frac{h^2}{4}V(x)\sin^2(\frac{kx}{2})} \tag{63}$$

2.2 b

Use Crank-Nicolson for the time integration and central differencing for spatial discretization to solve the Schrödinger equation. Write down the numerical scheme explicitly.

2.2.1 Solution

Using central differencing,

$$\frac{\partial^2\psi}{\partial x^2}(x,t) \approx \frac{\psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)}{a^2} \tag{64}$$

$$\xi(x,t) = \frac{1}{i}\left[\frac{\psi(x+a,t) + \psi(x-a,t) - 2\psi(x,t)}{a^2} + V(x)\psi(x,t)\right] \tag{65}$$

Defining Crank-Nicolson with $\chi = \frac{\partial\phi}{\partial t}$:

$$\phi(t+h) - \frac{h}{2}\chi(t+h) = \phi(t) + \frac{h}{2}\chi(t) \tag{66}$$

We get:

$$\psi(x,t+h) - \frac{h}{2}\xi(t+h) = \psi(x,t) + \frac{h}{2}\xi(t) \tag{67}$$

$$\psi(x,t+h) - \frac{h}{2}\frac{1}{i}\left[\frac{\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)}{a^2} + V(x)\psi(x,t+h)\right] \tag{68}$$

$$= \psi(x,t) + \frac{h}{2i}\left[\frac{\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)}{a^2} + V(x)\psi(x,t)\right] \tag{69}$$

$$\psi(x,t+h)\left(1 - \frac{h}{2i}V(x)\right) - \frac{h}{2i}\left[\frac{\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)}{a^2}\right] \tag{70}$$

$$= \psi(x,t)\left(1 + \frac{h}{2i}V(x)\right) + \frac{h}{2i}\left[\frac{\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)}{a^2}\right] \tag{71}$$

This full expression is quite long, so let us define $P(x,t) = \left[\frac{\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)}{a^2}\right]$. This lets us write:

$$\psi(x,t+h)\left(1 + \frac{h}{2i}V(x)\right) - \frac{h}{2i}P(x,t+h) = \psi(x,t)\left(1 + \frac{h}{2i}V(x)\right) + \frac{h}{2i}P(x,t) \tag{72}$$

which doesn't really help us with computation, but with digestibility and understandability.

2.3 c

Implement the numerical method with the following parameters: $L = 10, x_0 = -5, \sigma = 1, k_0 = 5$, and three different values for the energy barrier $V_0 = 0, k_0^2, 2k_0^2$. Plot a **kymograph** of the probabilty density $|\psi(x,t)|^2$ for $t \in [0,5]$ and $x \in [-L, L]$. Note: a **kymograph** is a space-time plot where the horizontal axis represents space, (here, x), the vertical axis represents time (here, t), and the color or brightness encodes the value of a quantity–in this case, the probability density$|\psi(x,t)|^2$. Plot the probability of being on the left or right side of the barrier $P(x<0,t) = \int_{-L}^{0} x\psi^*(x,t)\psi(x,t)dx$ and $P(x>0,t) = \int_0^L x\psi^*(x,t)\psi(x,t)dx$. Plot the mean position $\bar{x}(t) = \int_{-L}^{L} x\psi^*(x,t)\psi(x,t)dx$ for all three cases on the same graph. Breifly comment on how the step height V_0 affects the transmission and reflection of the wavepacket.

2.3.1 Solution

See problem2c.py and run with ‘python problem2c.py‘.

2.3.2 Comment

As V_0 increases, the ratio of transmission to reflection trends from 1 to zero.

2.4 d(Bonus)

Prove that Crank-Nicolson conserves probability. Specifically, show that for any Hamiltonian $\mathcal{H}$, using the following numerical scheme,

$$i(\psi(t+h) - \psi(t)) = \frac{h}{2}\mathcal{H}(\psi(t+h) + \psi(t)) \tag{73}$$

conserves the probablity, that is,

$$\langle\psi(t+h)|\psi(t+h)\rangle = \langle\psi(t)|\psi(t)\rangle \tag{74}$$

Or equivalently in vector notation,

$$\psi(t+h)^\dagger\psi(t+h) = \psi(t)^\dagger\psi(t) \tag{75}$$

Where † denotes the Hermitian conjugate (complex conjugate transpose) of the vector.
Then show that forward Euler and backward Euler schemes do not necessarily conserve probability.

2.4.1 Crank-Nicolson Preserves Probability

From the definition of Crank-Nicolson we have that,

$$|\psi(t+h)\rangle = \frac{i + \frac{hH}{2}}{i - \frac{hH}{2}}|\psi(t)\rangle \tag{76}$$

$$\langle\psi(t+h)| = \langle\psi(t+h)|\left(\frac{i + \frac{hH}{2}}{i - \frac{hH}{2}}\right)^* = \langle\psi(t+h)|\left(\frac{i - \frac{hH}{2}}{i + \frac{hH}{2}}\right) \tag{77}$$

$$\langle\psi(t+h)|\psi(t+h)\rangle = \langle\psi(t)|\frac{i - \frac{hH}{2}}{i + \frac{hH}{2}} \cdot \frac{i + \frac{hH}{2}}{i - \frac{hH}{2}}|\psi(t)\rangle = \langle\psi(t)|\psi(t)\rangle \tag{78}$$

Thus, Crank-Nicolson preserves probability.

2.4.2 Forward Euler Doesn't Preserve Probability

Forward Euler gives us:

$$\psi(t+h) = \psi(t) - ihH\psi(t) \tag{79}$$

$$|\psi(t+h)\rangle = (1 - ihH)|\psi(t)\rangle \tag{80}$$

$$\langle\psi(t+h)| = \langle\psi(t)|(1 + ihH) \tag{81}$$

$$\langle\psi(t+h)|\psi(t+h)\rangle = \langle\psi(t)|1 + h^2H^2|\psi(t)\rangle \neq \langle\psi(t)|\psi(t)\rangle \tag{82}$$

for $h, H|\psi(t)\rangle \neq 0$.

2.4.3 Backward Euler Doesn't Preserve Probability

Backwards Euler gives us:

$$|\psi(t+h)\rangle = \frac{1}{1-ihH}|\psi(t)\rangle \tag{83}$$

$$\langle\psi(t+h)| = \langle\psi(t)|\frac{1}{1+ihH} \tag{84}$$

$$\langle\psi(t+h)|\psi(t+h)\rangle = \langle\psi(t)|\frac{1}{1+h^2H^2}|\psi(t)\rangle \neq \langle\psi(t)|\psi(t)\rangle \tag{85}$$

for $h, H|\psi(t)\rangle \neq 0$.