Partial differential equations assignment

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Course: SS Physics

Computer simulation II

graphs for (c) and (d) attached at end of document

.py file attached separately

(a) $$i\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} = -\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2}$$

$$i\left(\frac{e_j^{n+1}-e_j^n}{\Delta t}\right) = -1\left(\frac{e_{j+1}^n - 2e_j^n + e_{j-1}^n}{\Delta x^2}\right)$$

$$e = A(t)e^{ikx}$$

$$e_j^{n+1} = A(t+\Delta t)\, e^{ikx}$$
$$e_i^n = A(t)\, e^{ikx}$$
$$e_{i+1}^n = A(t)\, e^{ik(x_i+\Delta x)}$$
$$e_i^n = A(t)\, e^{ikx_i}$$

$$e_{i-1}^n = A(t)\, e^{ik(x_i-\Delta x)}$$

$$i\left(\frac{A^{n+1}e^{ikx} - A^n e^{ikx}}{\Delta t}\right) = -\frac{A^n}{\Delta x^2}\left(e^{ik(x+\Delta x)} - 2e^{ikx} + e^{ik(x-\Delta x)}\right)$$

divide by $A^n e^{ikx}$

$$i\left(\frac{A^{n+1}}{A^n} - 1\right) = -\frac{\Delta t}{\Delta x^2}\left(e^{ik\Delta x} - 2 + e^{ik(-\Delta x)}\right)$$

$$\left(\sin\left(\frac{a}{2}\right)\right)^2 = \frac{1}{2}\left(1 - \cos(a)\right)$$

also noting $\cos k\Delta x = \dfrac{e^{ik\Delta x} + e^{-ik\Delta x}}{2}$

$$i\left(\frac{A^{n+1}}{A^n} - 1\right) = -\frac{2\Delta t}{\Delta x^2}\left(\cos(k\Delta x) - 1\right)$$

$$i\left(\frac{A^{n+1}}{A^n} - 1\right) = \frac{4\Delta t}{(\Delta X)^2}\left(\sin^2\left(\frac{k\Delta X}{2}\right)\right)$$

$$\frac{A^{n+1}}{A^n} = 1 - \frac{4i\Delta t}{\Delta X^2}\left(\sin^2\left(\frac{k\Delta X}{2}\right)\right)$$

The latter term will always be less than 1

$$|\varepsilon| < 1$$

$\therefore$ The scheme is stable unconditionally

$$|\varepsilon| = \sqrt{\left(1 - \frac{4\Delta t}{\Delta X^2}\left(\sin^2\frac{k\Delta X}{2}\right)\right)^2}$$

(b) $$i\frac{\psi_j^{n+1}-\psi_j^{n-1}}{2\Delta t} = -\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2}$$

$$\psi_j^{n+1} - \psi_j^{n-1} = 2i\Delta t\left(\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2}\right)$$

$$\gamma = \frac{i\Delta t}{\Delta x^2}$$

$$\psi_j^{n+1} = \psi_j^{n-1} + 2\gamma\left(\frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2}\right)$$

$$A^{n+1}e^{ikx} = A^{n-1}e^{ikx} + 2\gamma\left(A^n e^{ik(x+\Delta x)} - 2A^n e^{ikx} + A^n e^{ik(x-\Delta x)}\right)$$

$$A = A^{-1} + 2\gamma\left(e^{ik\Delta x} - 2 + e^{-ik\Delta x}\right)$$

$$A = A^{-1} + 4\gamma\left(\cos k\Delta x - 1\right)$$

$$A = A^{-1} - 8\gamma\sin^2\left(\frac{k\Delta x}{2}\right)$$

$$A = \frac{1}{A} - 8\gamma\left(\sin^2\left(\frac{k\Delta x}{2}\right)\right)$$

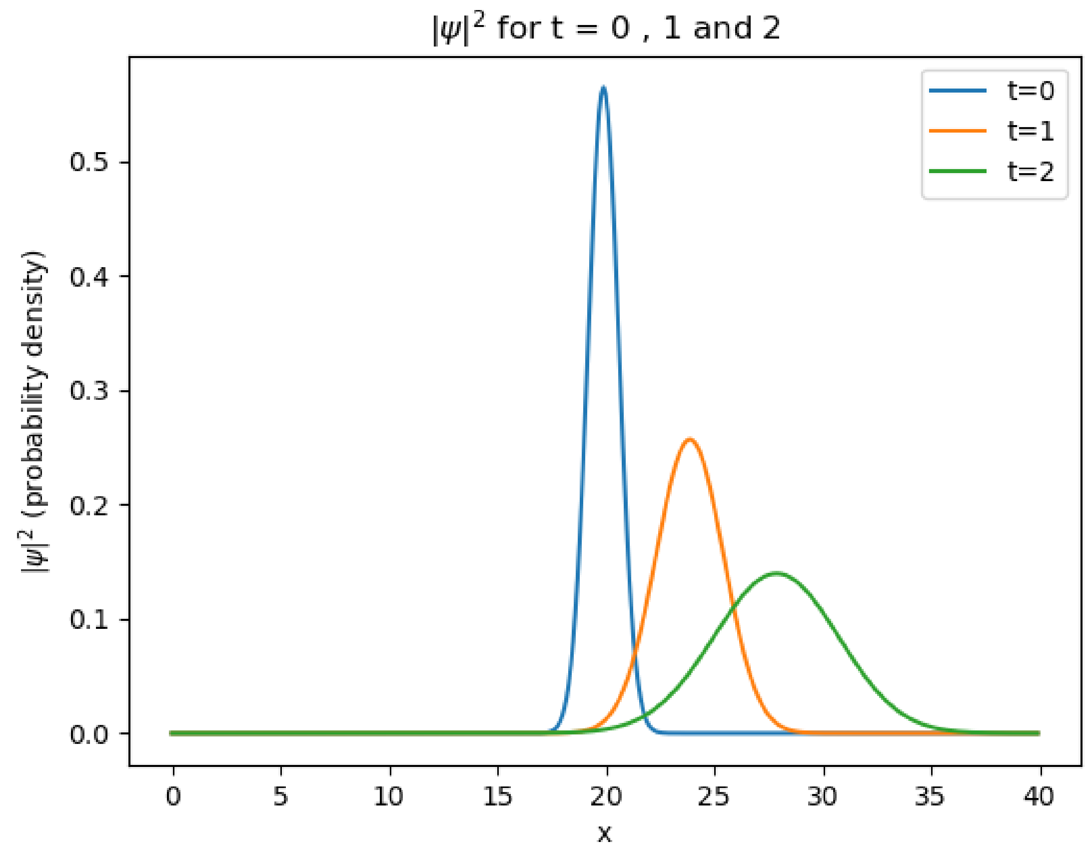
$$A^2 + A\left(8\gamma\sin^2\left(\frac{k\Delta x}{2}\right)\right) - 1 = 0$$

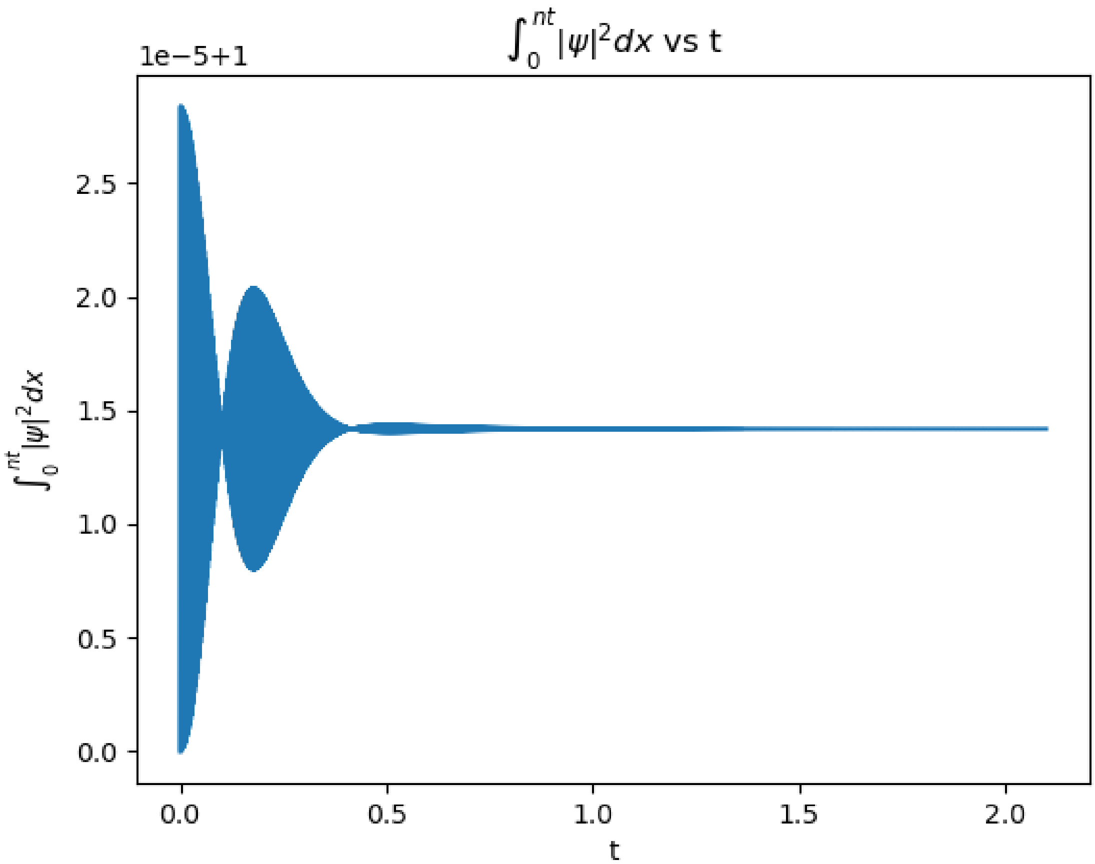
(e) The wave function converges to a simple form related to the momentum distribution of the packet. The wave is asymptotic and the probability distribution becomes static, though the scale increases linearly with time.

(d) see attached graph

This finite difference scheme is only suitable for short time durations as can be seen from how $\int|\psi|^2 dx$ becomes static

(c) at times $t=0$, $t=1$ and $t=2$ the wave spreads out and the peak decreases in height. The wavepacket disperses


$|\psi|^2$ for t = 0 , 1 and 2
t=0
t=1
t=2
0.5
0.4
0.3
0.2
0.1
0.0
$|\psi|^2$ (probability density)
0
5
10
15
20
25
30
35
40
x



$\int_0^{nt} |\psi|^2 dx$ vs t
1e−5+1
2.5
2.0
1.5
1.0
0.5
0.0
$\int_0^{nt} |\psi|^2 dx$
0.0
0.5
1.0
1.5
2.0
t