HW

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Problem 1

(a) In this part we use the fact

$$\int_{-\infty}^{\infty} \exp\bigl(-ax^2 + bx\bigr)dx = \left(\frac{\pi}{a}\right)^{1/2} \exp\left[\frac{b^2}{4a}\right]$$

Take the Fourier transform of the PDE in x, using the fact $\widehat{\partial_x^n \psi} = (i\xi)^n \psi$.

$$\hat{\psi}_t = \frac{i}{2}(i\xi)^2\hat{\psi} = -\frac{i}{2}\xi^2\hat{\psi} \implies \hat{\psi}(\xi, t) = \hat{\psi}_0(\xi)\exp\left[-\frac{i}{2}\xi^2 t\right]$$

Take the inverse Fourier transform.

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \hat{\psi}_0(\xi)\exp\left[ix\xi - \frac{i}{2}t\xi^2\right]d\xi$$

Take the Fourier transform of the initial condition.

$$\begin{aligned}
\hat{\psi}_0(\xi) &= \frac{1}{(2\pi)^{1/2}}\frac{1}{(2\pi\sigma_0^2)^{1/4}}\int_{-\infty}^{\infty}\exp\left[-\frac{x^2}{4\sigma_0^2} + ik_0x - i\xi x\right]dx \\
&= \frac{1}{(2\pi)^{3/4}\sigma_0^{1/2}}\int_{-\infty}^{\infty}\exp\left[-\frac{x^2}{4\sigma_0^2} + i(k_0 - \xi)x\right]dx \\
&= \frac{1}{(2\pi)^{3/4}\sigma_0^{1/2}}\pi^{1/2}2\sigma_0\exp\bigl[-(\xi - k_0)^2\sigma_0^2\bigr] \\
&= \frac{2^{1/4}\sigma_0^{1/2}}{\pi^{1/4}}\exp\bigl[-(\xi - k_0)^2\sigma_0^2\bigr]
\end{aligned}$$

Then

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}}\frac{2^{1/4}\sigma_0^{1/2}}{\pi^{1/4}}\int_{-\infty}^{\infty}\exp\left[-\sigma_0^2(\xi - k_0)^2 - \frac{i}{2}t\xi^2 + ix\xi\right]d\xi$$

Rewrite the argument of exp as

$$-\sigma_0^2(\xi - k_0)^2 - \frac{i}{2}t\xi^2 + ix\xi = -\sigma_0^2(\xi^2 + k_0^2 - 2k_0\xi) - \frac{i}{2}t\xi^2 + ix\xi = -\left(\sigma_0^2 + \frac{i}{2}t\right)\xi^2 + (ix + 2\sigma_0^2k_0)\xi - \sigma_0^2k_0^2$$

so that

$$\begin{aligned}
\psi(x,t) &= \frac{\sigma_0^{1/2}}{2^{1/4}\pi^{3/4}} \int_{-\infty}^{\infty} \exp\left[-\left(\sigma_0^2 + \frac{i}{2}t\right)\xi^2 + (ix + 2\sigma_0^2 k_0)\xi - \sigma_0^2 k_0^2\right] d\xi \\
&= \frac{\sigma_0^{1/2}}{2^{1/4}\pi^{3/4}} e^{-\sigma_0^2 k_0^2} \left(\frac{\pi}{\sigma_0^2 + \frac{i}{2}t}\right)^{1/2} \exp\left[\frac{-x^2 + 4\sigma_0^4 k_0^2 + 4i\sigma_0^2 k_0 x}{4\left(\sigma_0^2 + \frac{i}{2}t\right)}\right] \\
&= \frac{\sigma_0^{1/2} e^{-\sigma_0^2 k_0^2}}{2^{1/4}\pi^{1/4}} \left(\sigma_0^2 + \frac{i}{2}t\right)^{-1/2} \exp\left[\frac{-x^2 + 4\sigma_0^4 k_0^2 + 4i\sigma_0^2 k_0 x}{4\left(\sigma_0^2 + \frac{i}{2}t\right)}\right]
\end{aligned}$$

(b) Discretize the PDE in space with stepsize h and use central differences.

$$\psi_j'(t) = \frac{i}{2h^2}[\psi_{j+1}(t) + u_{j-1}(t) - 2u_j(t)]$$

Let v be such that $v(x_j, t) = \psi_j(t)$.

$$v_t(x,t) = \frac{i}{2h^2}[v(x+h,t) + v(x-h,t) - 2v(x,t)]$$

Taylor expand.

$$\begin{aligned}
v(x+h,t) &= v + hv_x + \frac{1}{2}h^2 v_{xx} + \frac{1}{6}h^3 v_{xxx} + \frac{1}{24}h^4 v_{xxxx} + \frac{1}{120}h^5 v_{xxxxx} + O(h^6) \\
v(x-h,t) &= v - hv_x + \frac{1}{2}h^2 v_{xx} - \frac{1}{6}h^3 v_{xxx} + \frac{1}{24}h^4 v_{xxxx} - \frac{1}{120}h^5 v_{xxxxx} + O(h^6)
\end{aligned}$$

Plug in.

$$v_t = \frac{i}{2h^2}\left[h^2 v_{xx} + \frac{1}{12}h^4 v_{xxxx} + O(h^6)\right] = \frac{i}{2}v_{xx} + \frac{i}{24}h^2 v_{xxxx} + O(h^4)$$

We obtain the (third order) modified equation.

$$v_t - \frac{i}{2}v_{xx} = \frac{i}{24}h^2 v_{xxxx}$$

The Fourier transform of the RHS term is

$$\frac{i}{24}h^2\xi^4\hat{v}$$

so its corresponding term within the solution $\hat{v}(\xi, t)$ in Fourier space is

$$\exp\left[\frac{i}{24}h^2\xi^4 t\right]$$

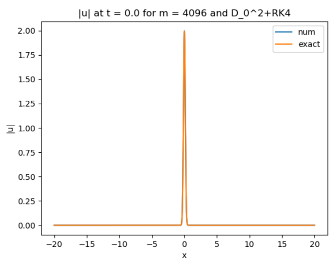
Thus the modified equation introduces artificial Fourier modes which do not decay over time.

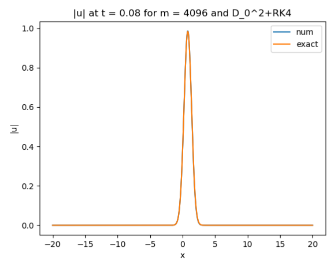
(c) pick maximum time T
pick stepsize h and timestep k
set mesh using stepsize h
$N \leftarrow \frac{T}{k}$
set time points between 0 and T using timestep k
set initial condition vector u_0
$\hat{u}_0 \leftarrow$ DFT of u_0
$\xi \leftarrow 2\pi$ times vector of wavenumbers corresponding to mesh
$\hat{u} \leftarrow$ solution of PDE in Fourier space, $\hat{u}_t = -\frac{i}{2}\xi^2\hat{u}$ (use SciPy solver with $\hat{u}_0$ and set of time points)
$u \leftarrow$ array of 0s with the same size as $\hat{u}$

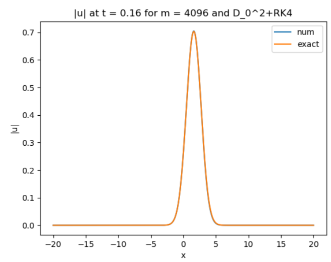
for jth row of u **do**
  set the jth row of u as the inverse DFT of the jth row of $\hat{u}$
end for
for $j = 0, \ldots, N$ **do**
  if $jk \in [0, t_1, \ldots, t_M]$ **then**
    print jth row of u
  end if
end for

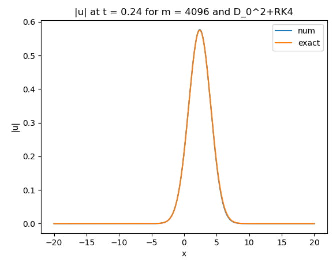
Problem 2

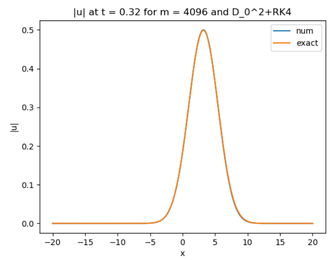
(a) In this part we take 4096 points in space. For D_0^2+RK4:

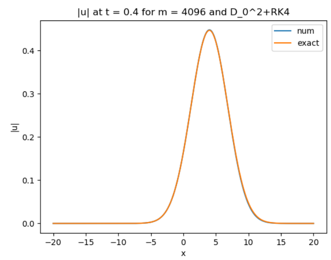




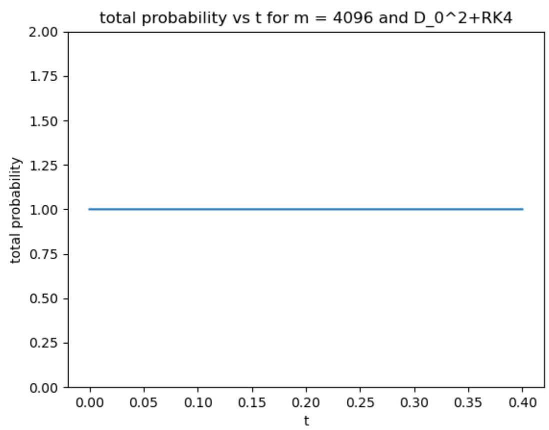




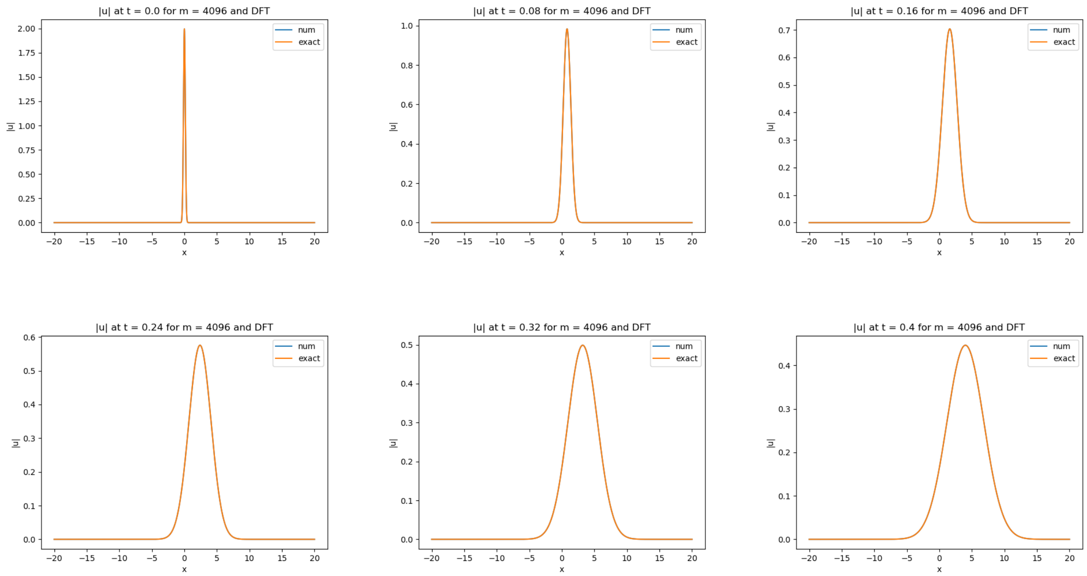




We check the total probability is nearly equal to 1.



For the method using the discrete Fourier transform (DFT):



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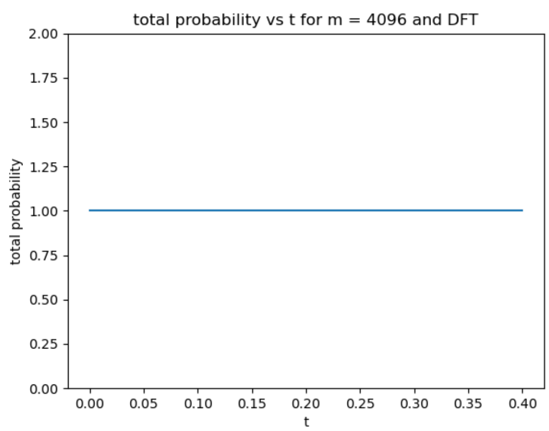
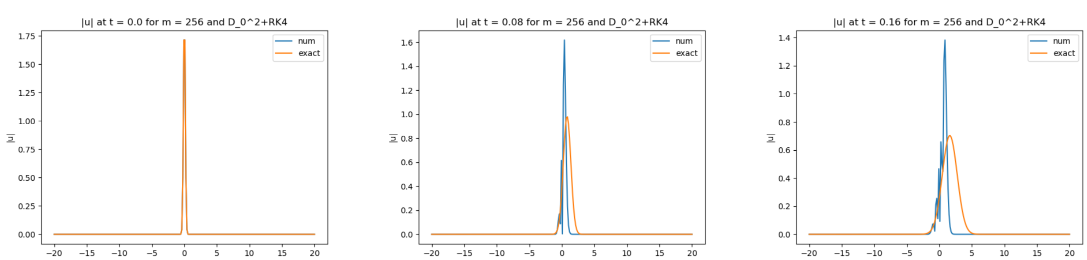
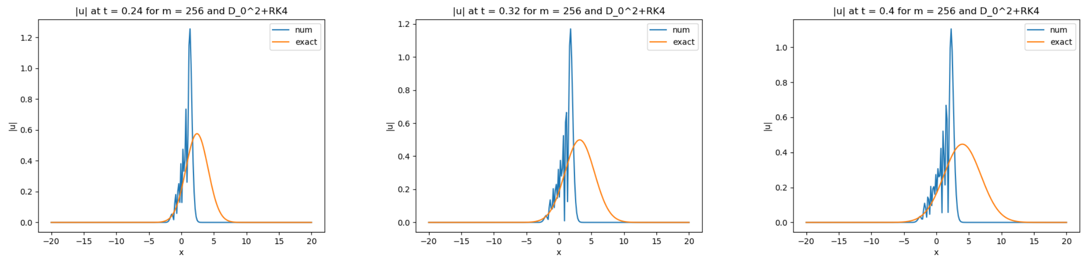


(b) In this part we take 256 points in space. For D_0^2+RK4:





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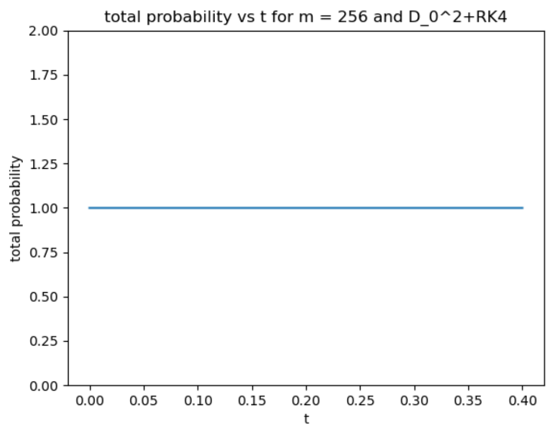

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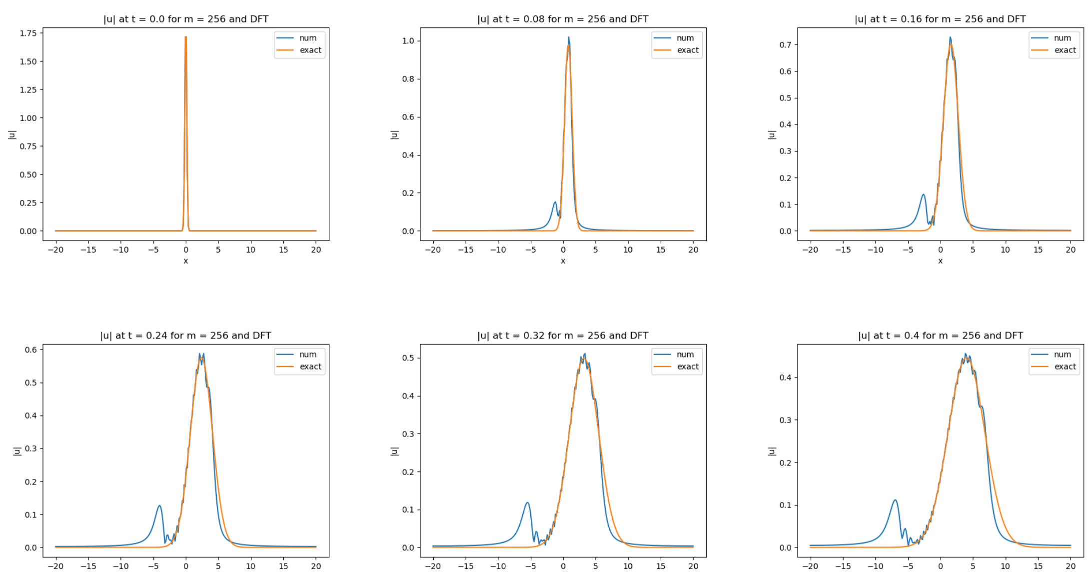

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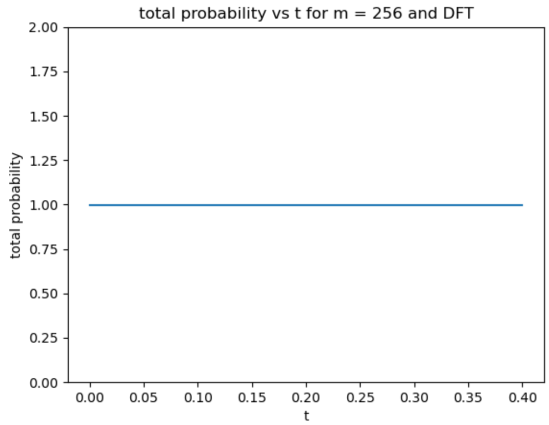

Problem 3

(a) Fix a test function $v \in H_0^1(\Omega)$. Multiply the PDE by v and integrate over Ω.

$$\int_\Omega \epsilon v \Delta u dx = \int_\Omega (u^3 - u) v dx$$

Using Green's first identity and the fact $v = 0$ on $\partial\Omega$, the LHS is

$$\int_\Omega \epsilon v \Delta u dx = -\int_\Omega \epsilon \nabla u \cdot \nabla v dx + \int_{\partial\Omega} \epsilon v \frac{\partial u}{\partial n} ds = -\int_\Omega \epsilon \nabla u \cdot \nabla v dx$$

Then we obtain the weak formulation.

$$-\int_\Omega \epsilon \nabla u \cdot \nabla v dx = \int_\Omega (u^3 - u) v dx \implies \int_\Omega \epsilon \nabla u \cdot \nabla v dx - \int_\Omega (u - u^3) v dx = 0$$

(b) e

(c) Code for problem 3:

`https://github.com/RokettoJanpu/Scientific-Computing-2/blob/main/FINAL%20q3.ipynb`

Below is a mesh of Ω.