Methods of Computational Physics

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January 4^{th}, 2020

Partial Differential Eqautions

a) The imaginary time Scrödinger equation - $-\frac{d\psi}{dt} = -\frac{h^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$, where $V = \frac{L^2}{2X_o^2\pi}\cos^2(\frac{\pi x}{L})$
Rewriting it in dimensionless form, using - $\frac{X}{X_o} = \tilde{X}, X_o^2 = \frac{h}{m\omega}$ and $\tau = \hbar\omega t$

$$\frac{\partial\psi}{\partial\tau} = \frac{1}{2}\frac{\partial^2\psi}{\partial\tilde{x}^2} - \frac{1}{2}[(\frac{L}{x_o\pi}\cos(\frac{\pi\tilde{x}x_o}{L}))^2 - \tilde{E_T}]\psi$$

where $\tilde{E} = \frac{E}{\hbar\omega}$.
Critical value E* as $\frac{L}{X_o} \longrightarrow \infty$ can be estimated to be equivalent to $\frac{1}{2}(\frac{L}{\pi x_o})^2$ without any calculation.
As $\tau \to \infty$, $\frac{L}{X_o} \to \infty$, the wave function limits to a gaussian.

b) Defining a tridiagonal matrix -

$$A = \begin{pmatrix} -2 & 1 & 0 & . & . & . & . & 1 \\ 1 & -2 & 1 & 0 & . & . & . & 0 \\ 0 & 1 & -2 & 1 & 0 & . & . & 0 \\ . & 0 & 1 & -2 & 1 & 0 & . & 0 \\ . & . & 0 & 1 & -2 & 1 & 0 & 0 \\ . & . & . & 0 & 1 & -2 & 1 & 0 \\ . & . & . & . & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & . & . & 0 & 1 & -2 \end{pmatrix} \text{ and } \beta = D\frac{\Delta t}{\Delta x^2}$$

I initialize my wavefunction with a delta function, initially, - $\delta(x - L/2)$. With L=20x_o and discretizing space into 200 grid points, I propagate my wavefunction for a $\tau_{fin} = 200$ using 3 methods -

- Forward Euler - $\psi(x, t+1) = (I + \beta A - I.V)\psi(x, t)$, where I is an identity matrix of the dimensions of A (200x200).
- Crank-Nicolson - $\psi(x, t+1) = (I - \frac{\beta A}{2})^{-1}(I + \frac{\beta A}{2} - I.V)\psi(x, t)$
- Pseudo-spectral - $\psi(x, t+1) = \exp(\frac{-V(x)\Delta t}{2})FFT_x^{-1}[\exp(-Dq^2\Delta t)FFT_q[\exp(\frac{-V(x)\Delta t}{2})\psi(x, t)]]$

Method	Δt	E_T
F. Euler	0.0091	0.499068233535
C. Nicolson	0.1	0.499068233535
Pseudo sp.	1	0.079898

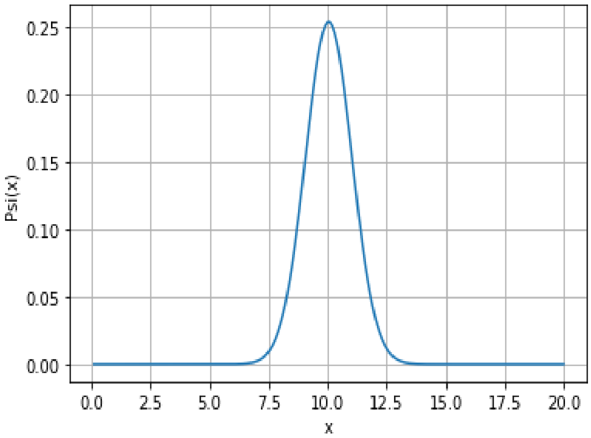

Figure 1: Wavefunction at the t=τ_{fin}

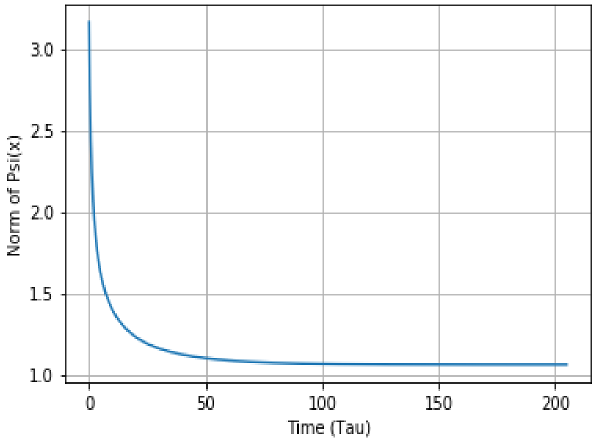

Figure 2: Stability of the norm of Psi(x)

Euler Forward

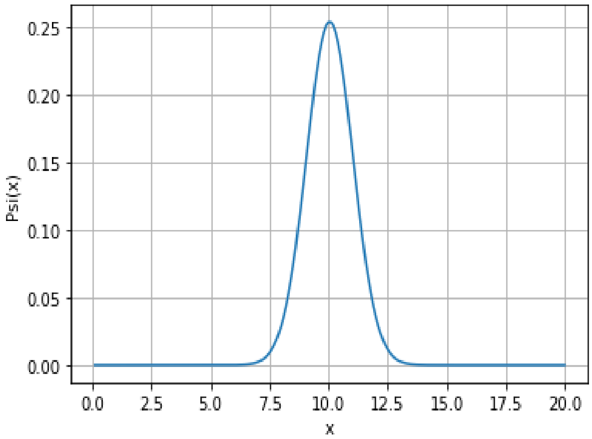

Figure 3: Wavefunction at the t=τ_{fin}

Crank-Nicolson

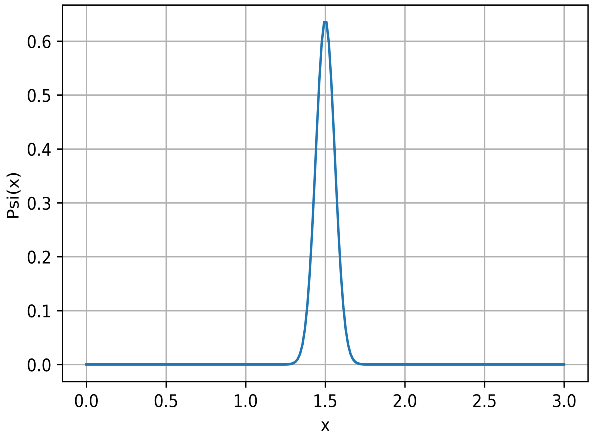

Figure 4: Wavefunction at the t=τ_{fin}

Pseudo-spectral

c) For L=3x_o, width of the wavefunction is more broad in comparison to L=20x_o

Method	Δt	E_T
F. Euler	0.0022	0.216780
C. Nicolson	0.1	0.216780
Pseudo sp.	1	0.070381

Above table depicts parameters for $\tau_{fin} = 200$

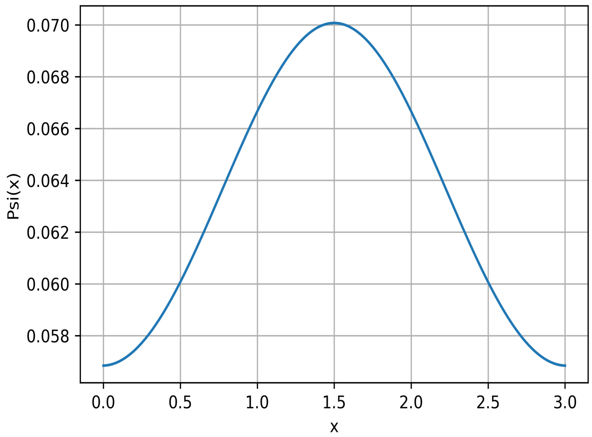

Figure 5: Wavefunction at the t=τ_{fin}

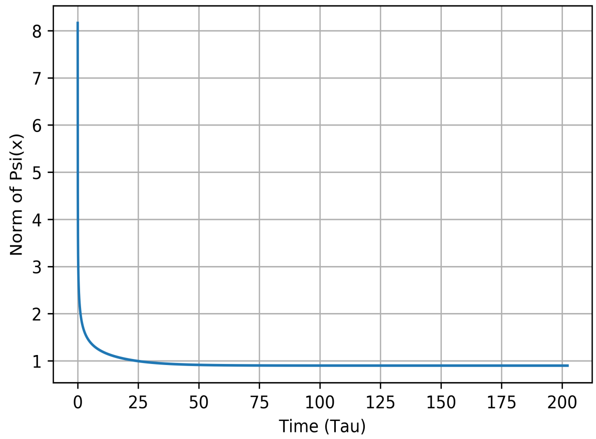

Figure 6: Stability of the norm of Psi(x)

L=3x$_o$

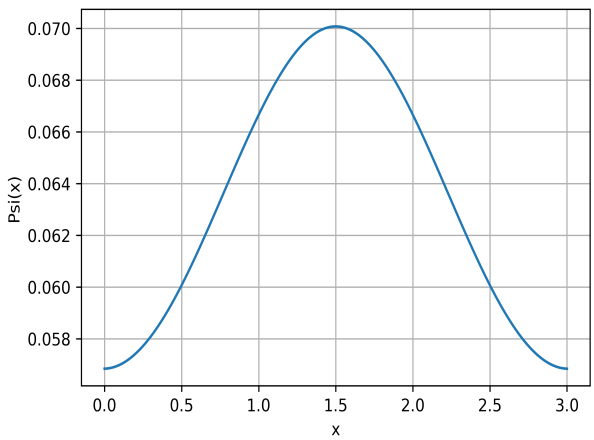

Figure 7: Wavefunction at the t=τ_{fin}

Crank-Nicolson

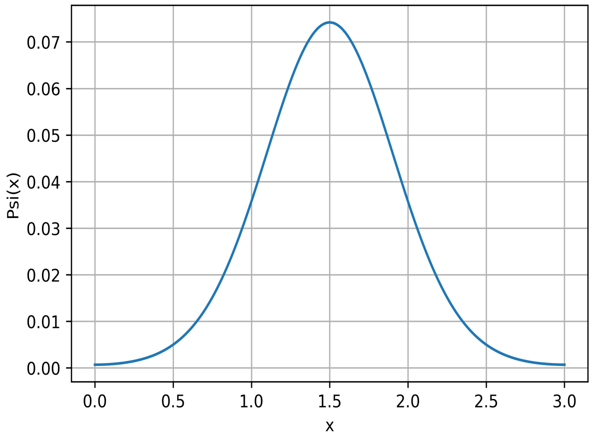

Figure 8: Wavefunction at the t=τ_{fin}

Pseudo-Spectral