A Numerical Approach to Solving the Time-Dependent Dirac Equation

(work in progress)

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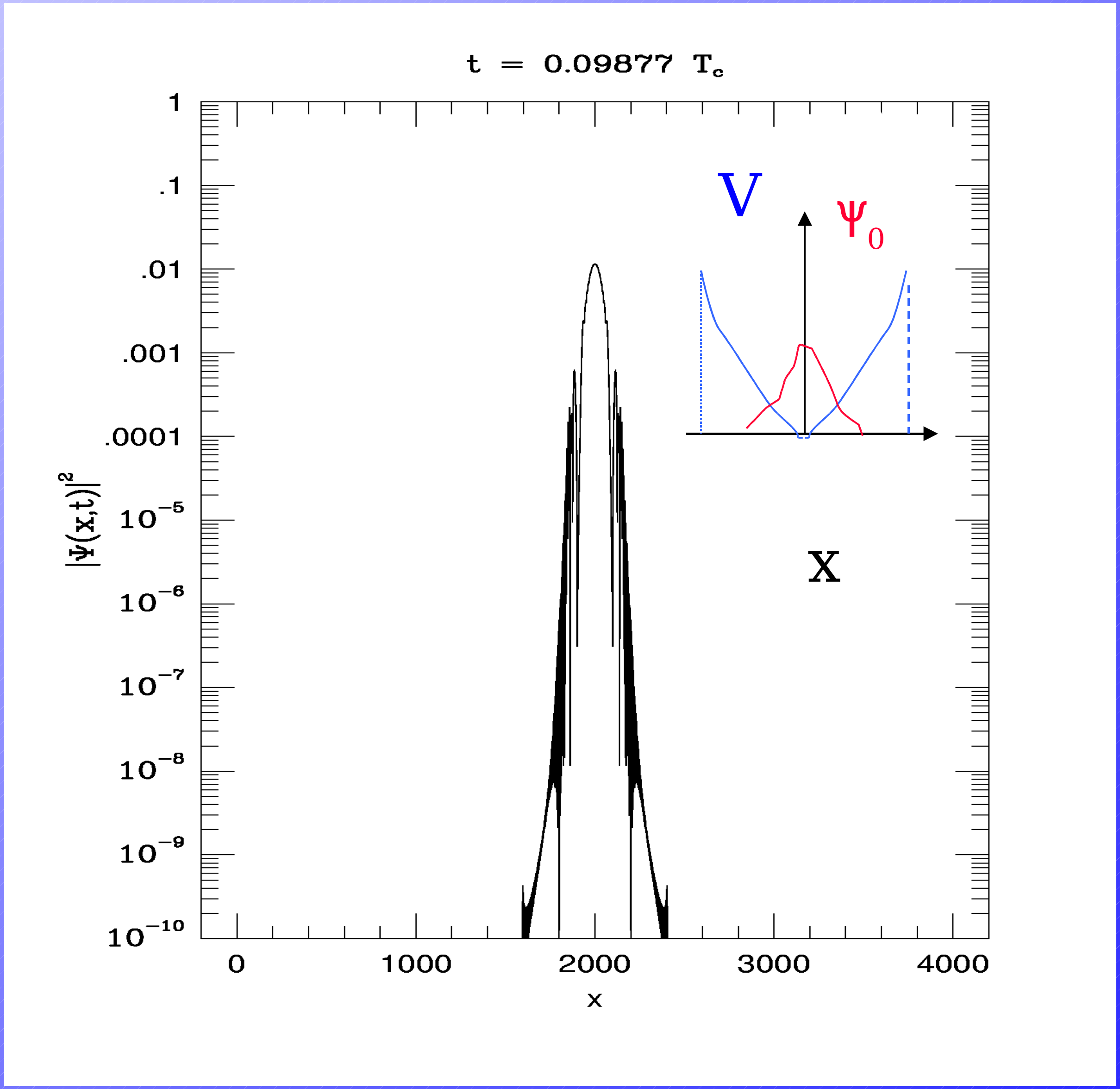
Staggered Leap-Frog Method

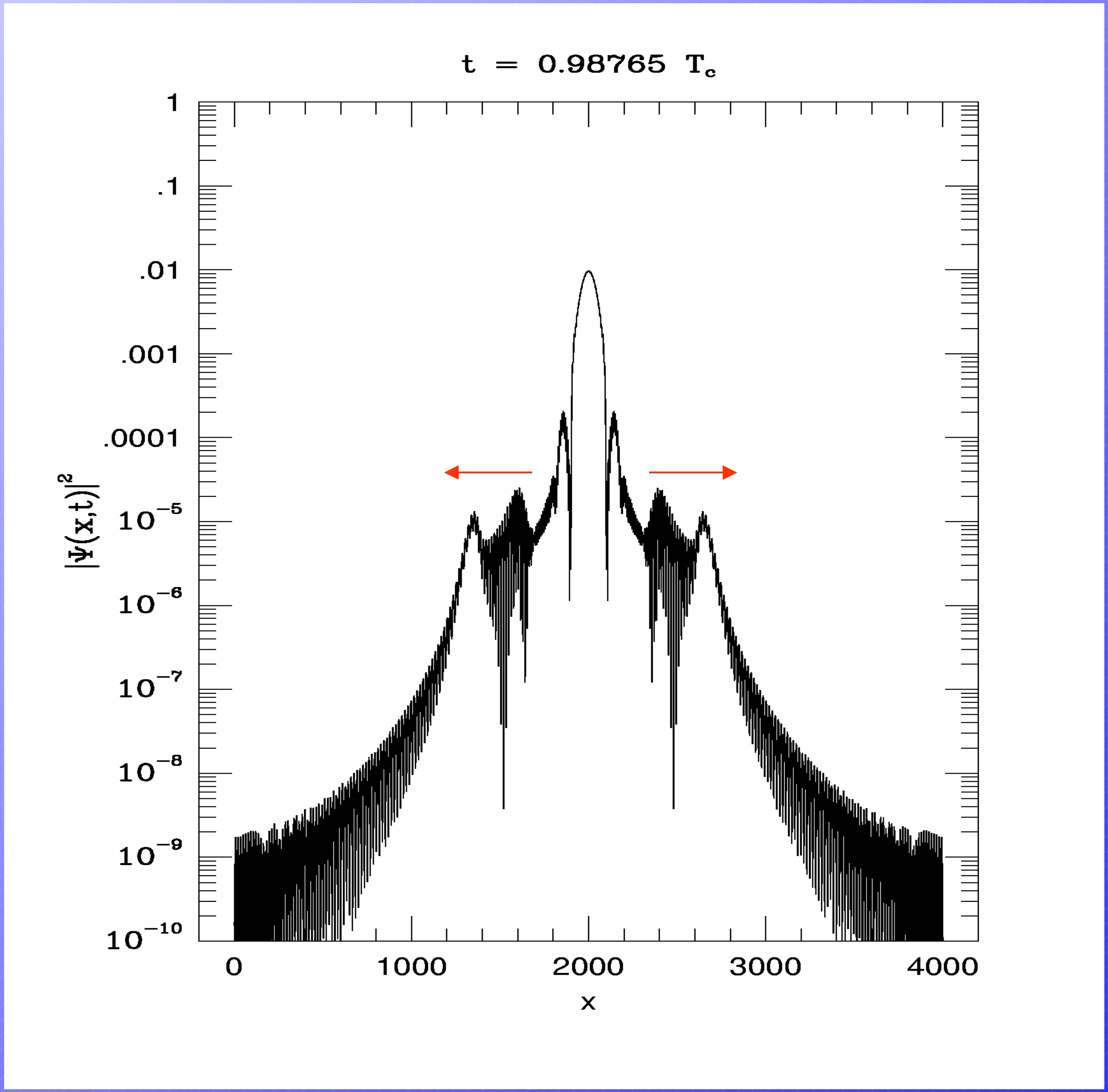
- Stable (checked vs analytical solutions and by calculating the norm)
- Accurate (error in $\Psi^{\dagger}\Psi \sim 10^{-9}$)
- Fast (Needs only desktop workstation)
- Spatial grid (up to 170^3)

$$\Psi_{(t+2dt)} = \Psi_{(t)} - i\hat{H}\Psi_{(t+dt)} 2dt$$

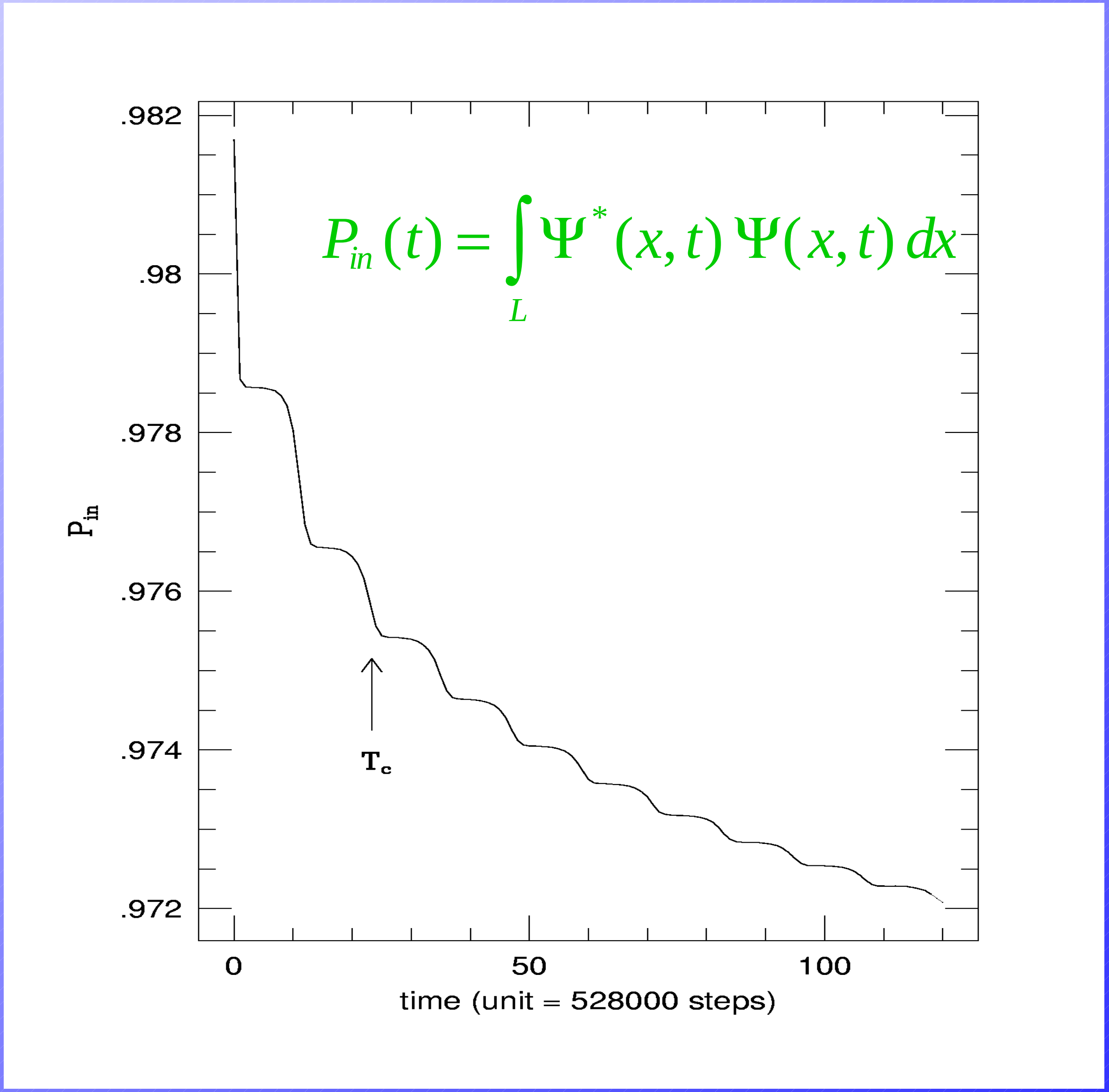
Previous Work with the Schrödinger Equation



Gaussian contained in finite well



Wave packet escapes



Non-exponential decay

J. W. Braun, Q. Su, R. Grobe [Phys. Rev. A 59, 604]

- Split-operator technique
- Zitterbewegung
- Klein Paradox
- Used a CRAY supercomputer

Dirac Free Hamiltonian

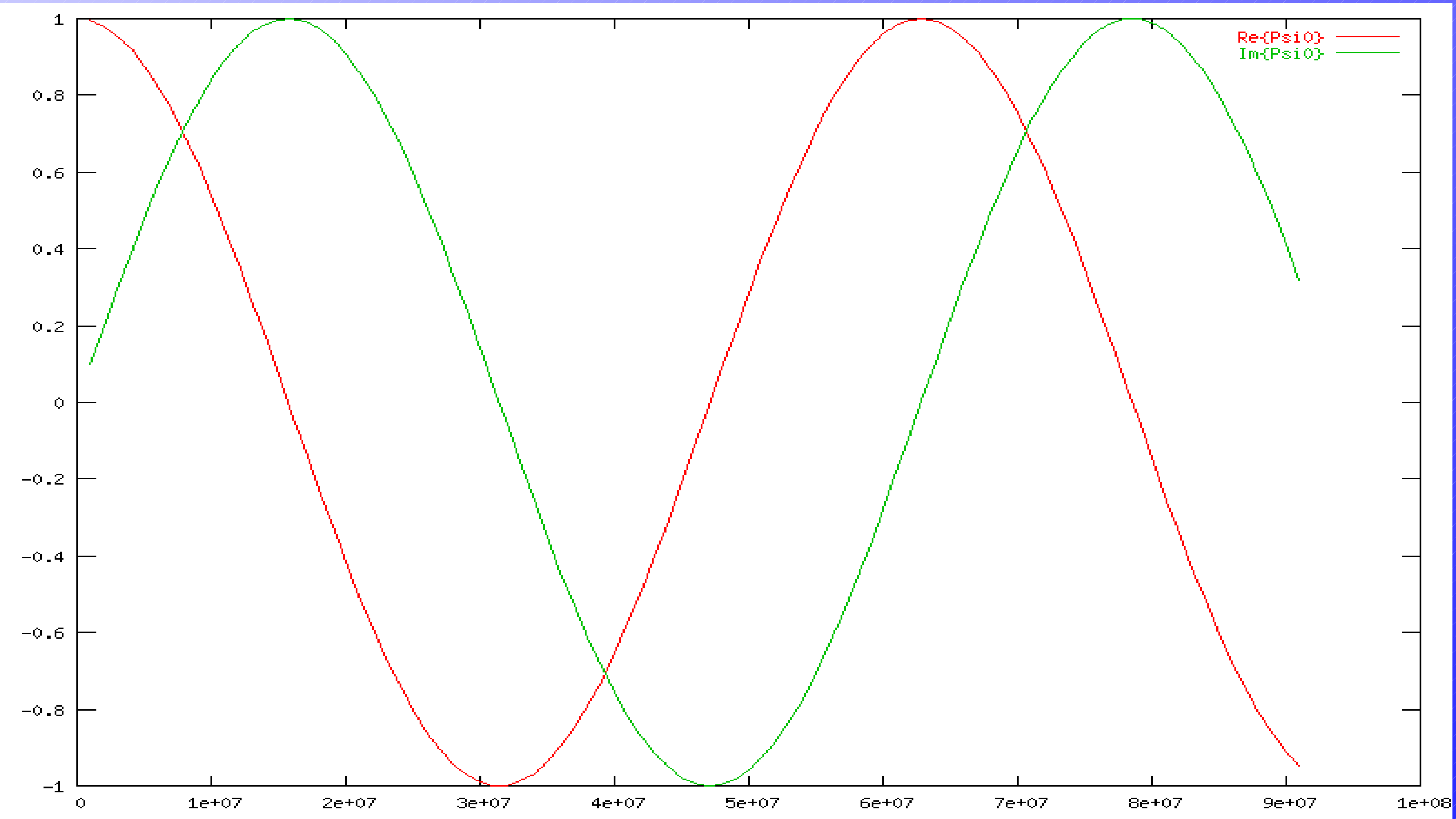
$$\left(\alpha_0 m c^2 + \sum_{j=1}^{3} \alpha_j \hat{p}_j c\right)\psi(\mathbf{x},t) = i\hbar \frac{\partial \psi}{\partial t}(\mathbf{x},t)$$

$$\begin{pmatrix} (\hat{p}_0 - mc) & 0 & -\hat{p}_3 & -(\hat{p}_1 - i\hat{p}_2) \\ 0 & (\hat{p}_0 - mc) & -(\hat{p}_1 + i\hat{p}_2) & \hat{p}_3 \\ -\hat{p}_3 & -(\hat{p}_1 - i\hat{p}_2) & (\hat{p}_0 + mc) & 0 \\ -(\hat{p}_1 + i\hat{p}_2) & \hat{p}_3 & 0 & (\hat{p}_0 + mc) \end{pmatrix} \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix} = 0$$

$$\hat{p}_j = -i\hbar \frac{\partial}{\partial x^j}$$

$$\hat{p}_0 = i\hbar \frac{\partial}{\partial_t}$$

Simple test Case



Time-step

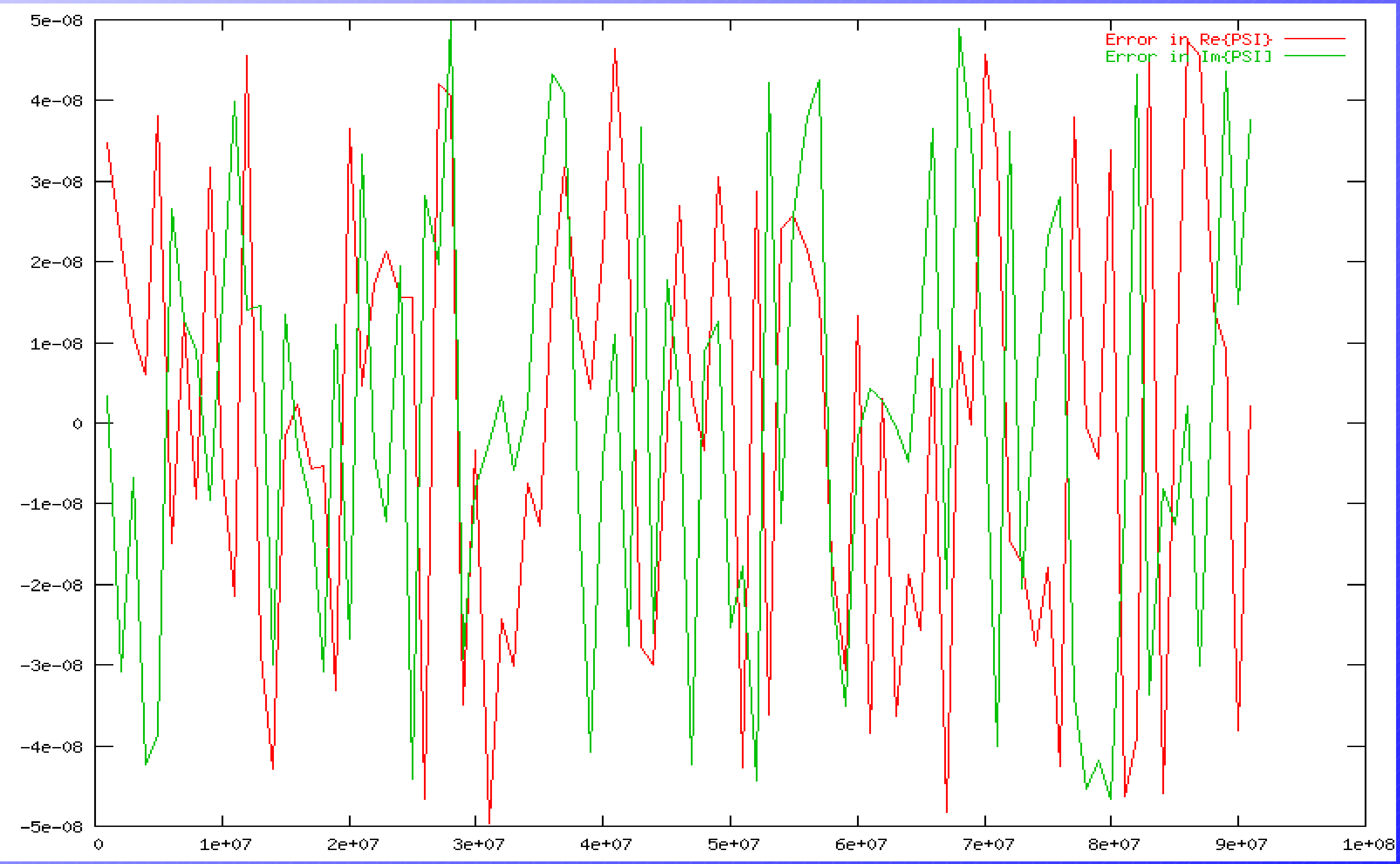
grid 90^3 points
$\Delta x = 0.05$
$\Delta t = 1 \times 10^{-7}$

Particle at Rest
Spin up E > 0

$$\Psi(\mathbf{x},t)=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}e^{-imt}$$

$$c=\hbar=1$$

Stability



Deviation from analytic
result vs time

Norm

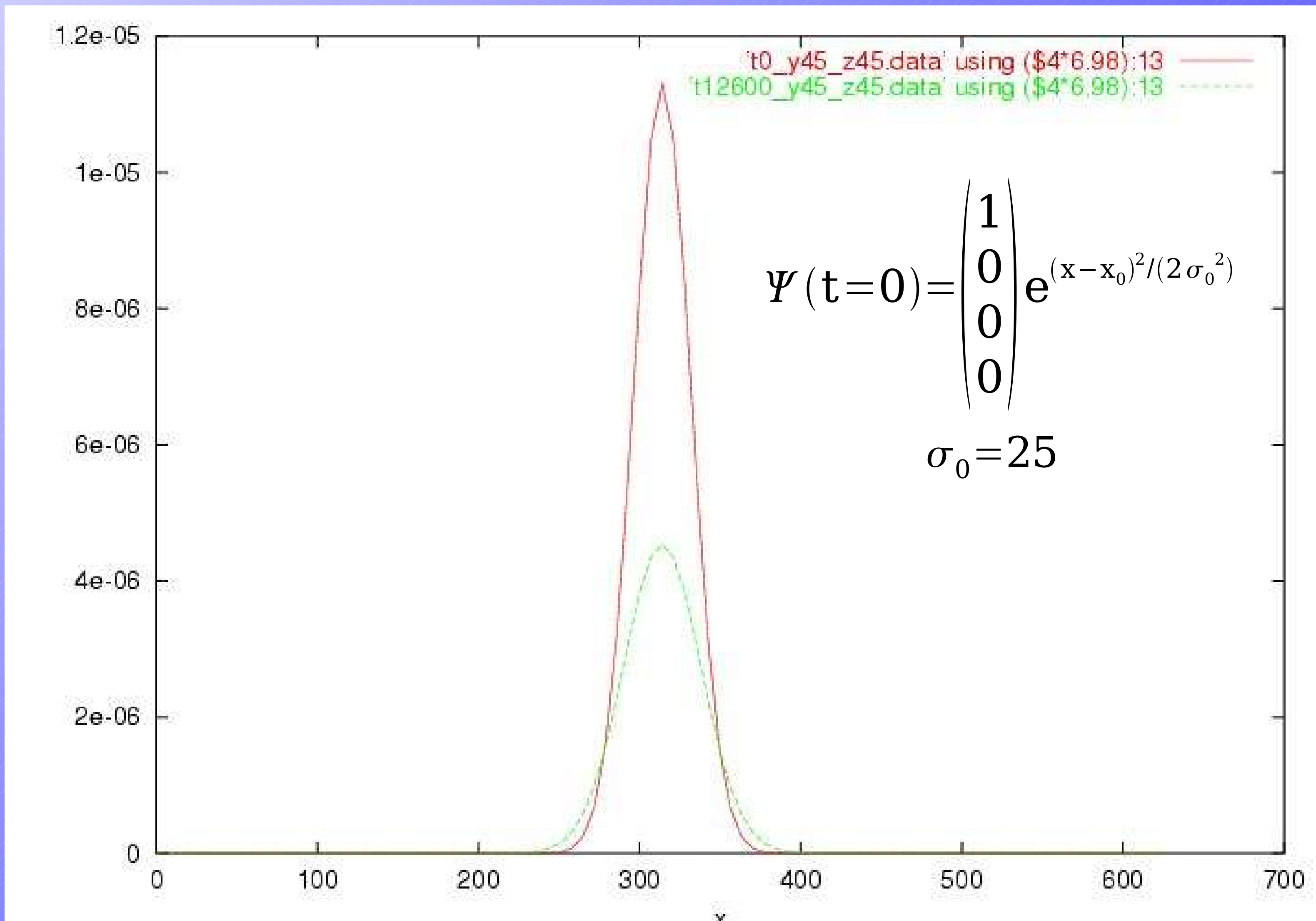
$$\int \Psi^\dagger \Psi \, d^3x = \text{Stable}$$

Eg.
$\Delta x = 6.98$
$\Delta t = 0.05$

Error in $N \sim 0.5\%$
Per point 10^{-9}

For stability: $\Delta t << \Delta x$ $(c=1)$

Stationary Gaussian



$$\Psi(t=0)=\begin{pmatrix}1\\0\\0\\0\end{pmatrix}e^{(x-x_0)^2/(2\sigma_0^2)}$$

$$\sigma_0=25$$

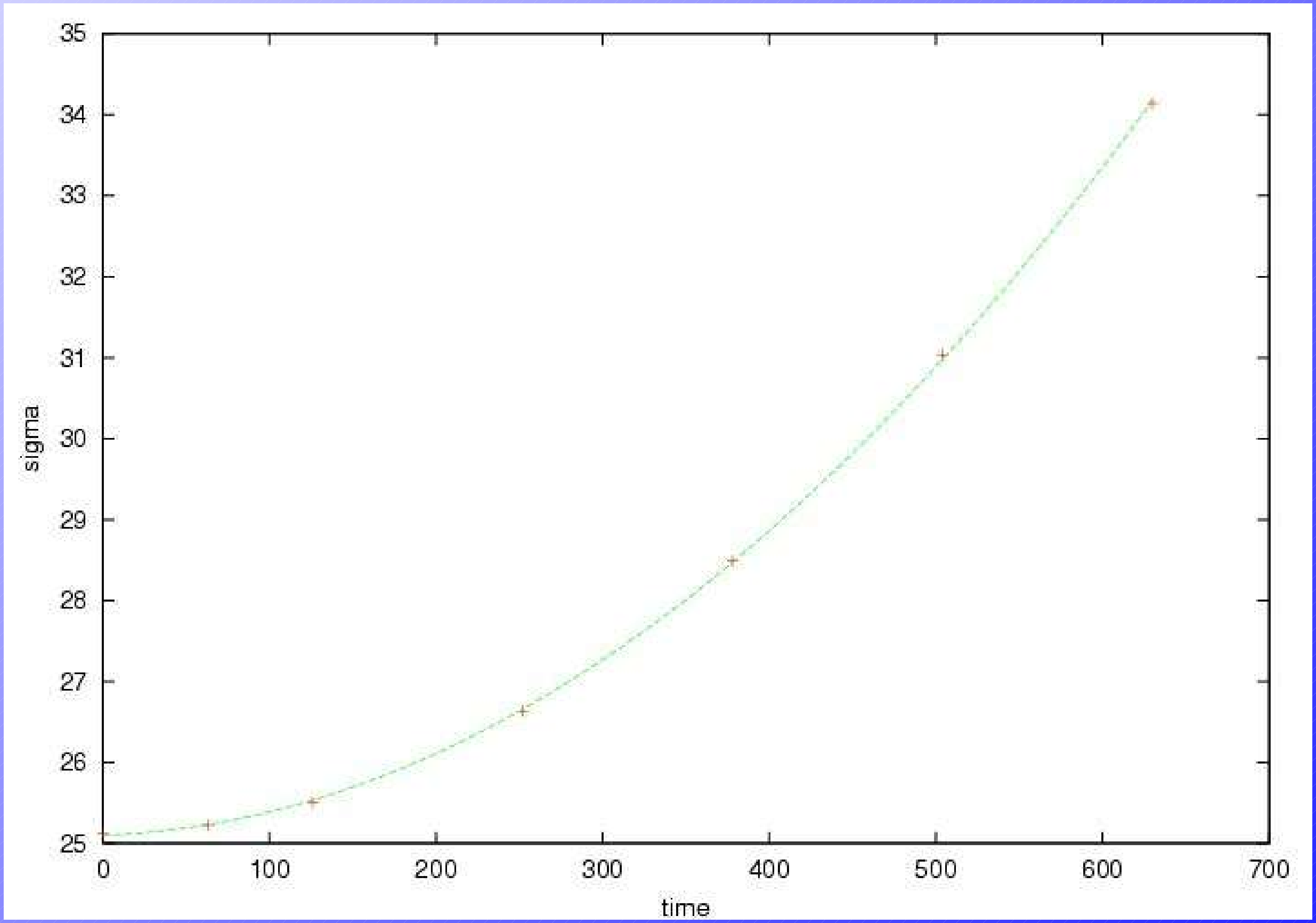
$\Delta x = 6.98$ $n=90^3$

$\Delta t = 0.05$ $L\approx 628$

It spreads!

$y=L/2$

$z=L/2$



σ increases ~ t^2

Zitterbewegung of Spin

$$\hat{S}_z(t) = \hat{S}_z + \frac{c}{2i}\left(e^{2i\hat{H}_0 t} - 1\right)\hat{H}_0^{-1}\alpha_y \hat{p}_x$$

Expected frequency $\omega = E \sim \sqrt{m^2 + k_0{}^2}$

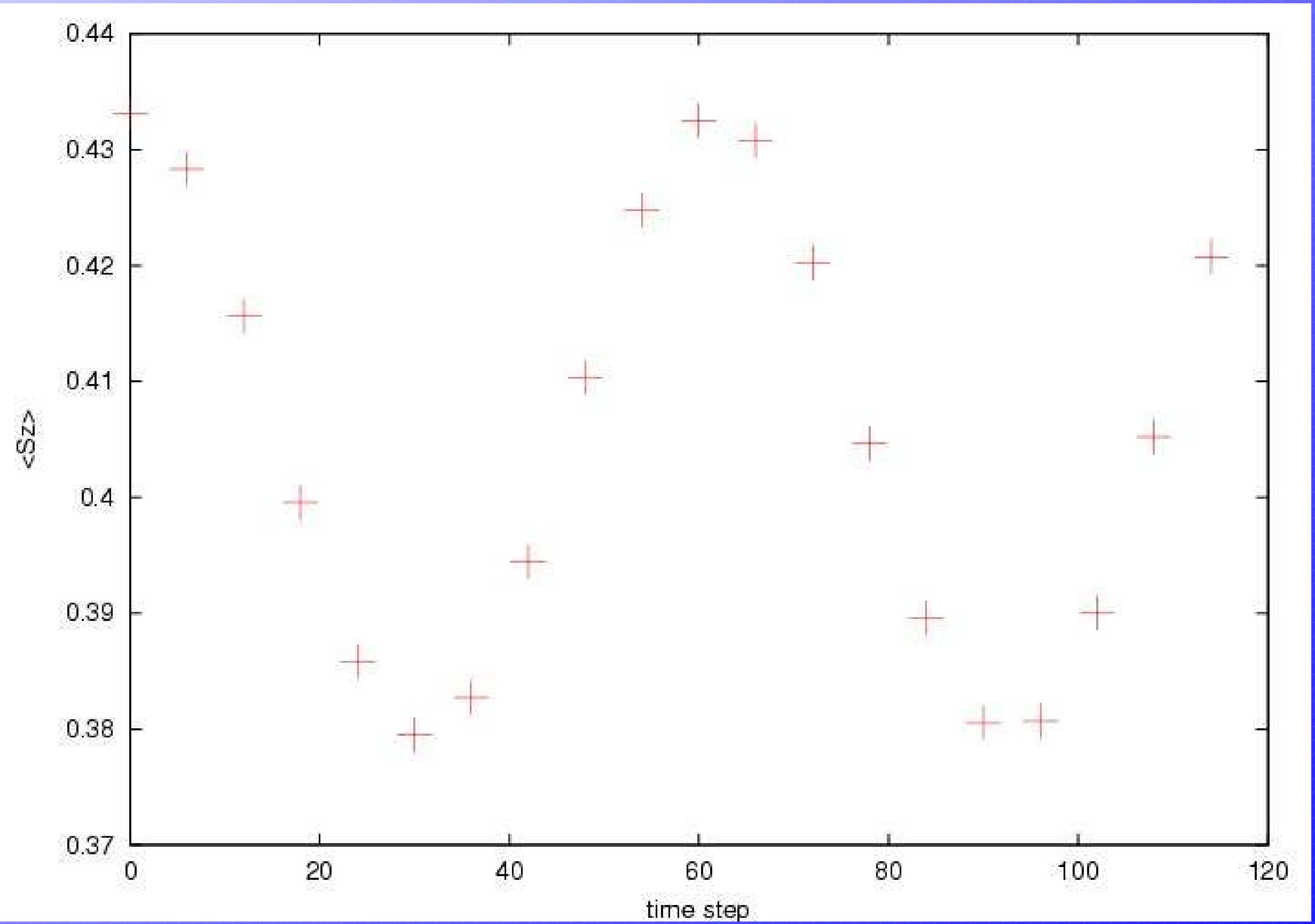
$$\langle S_z \rangle = \frac{1}{2}\left(\left|\Psi_0\right|^2 - \left|\Psi_1\right|^2 + \left|\Psi_2\right|^2 - \left|\Psi_3\right|^2\right)$$

Initial spin ≠ ½

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \dfrac{k_0}{1+\sqrt{1+k_0{}^2}} \end{pmatrix} e^{i k_0 x - (x - x_0)/2(\sigma)^2}$$

$$m = c = \hbar = 1$$

Zittergewegung of Spin



Future Plans

- Only a few attempts to solve Dirac Equation with arbitrary Ψ_0 and A^μ (minimal coupling)
- Study the Bohm-Aharonov Effect
- Introduce A^μ
  - Investigate relativistic non-exponential decay
  - Examine relativistic decay of mesons in medium