Numerical Resolution of the Schrödinger Equation

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Numerical Analysis Project, March 2011

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- Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r},t)\psi(\vec{r},t) = \mathrm{i}\hbar\partial_t\psi(\vec{r},t)$$

- Choice of units: $\hbar \equiv m \equiv 1$
- Choose a suitable numerical method
- Apply it on several physical problems

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1. Which numerical tools to choose ?
2. Cases in hand of Quantum Mechanics
3. Application to atomic and condensed matter physics

- In order to choose an appropriate method:
  - Look at the propagation of a Gaussian wave packet
  - Compare with the analytical solution
- 5 different algorithms
- Speed comparison between Matlab and C++

- Initial wave packet:

$$\psi(\vec{r}, t=0) = \mu \exp\left(-\frac{(\vec{r}-\vec{r_0})^2}{2\sigma^2}\right) \exp\left(\mathrm{i}\vec{k}\cdot\vec{r}\right)$$

- Norm $N(t)$ is set to 1
- Space and time are discretized
- The (unidimensionnal) Laplace operator becomes

$$\nabla^2\psi(x,t) \approx \frac{\psi(x+\Delta x, t) + \psi(x-\Delta x, t) - 2\psi(x,t)}{\Delta x^2}$$

Plot of $|\psi(x,t)|^2$ (blue: simulation, green: analytical solution)

(video missing)

- This result was obtained with a Runge Kutta 4 algorithm
- Discretization : $\Delta t = 0.0001$ and $\Delta x = 0.01$

Why did we choose Runge Kutta 4?

- We compared Runge Kutta 4 (RK4) to
  - forward Euler (Euler)
  - Crank-Nicholson (CN)
  - Runge Kutta 2 (RK2)
  - TR-BDF2

- Similar accuracy provided that discretization is small enough

- RK4 was the fastest method for a given accuracy
  Example for free propagation: 1.3 s for RK4 compared to 83 s for Euler

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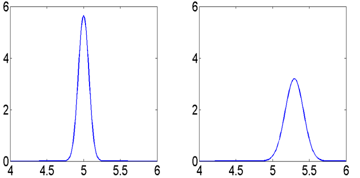
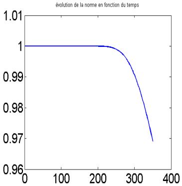
Which numerical tools to choose?

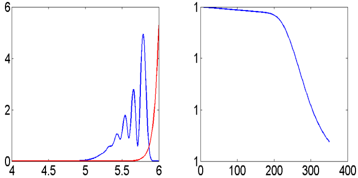
Reflexion of the wave packet on a barrier



$|\psi(x,t)|^2$ at time steps 1,150 and 350, with an infinite barrier



Loss of norm



With an exponential potential barrier

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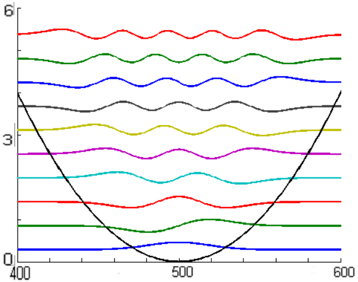
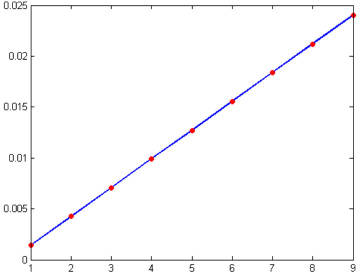
- Discretization: $\Delta x = 1$, $N_x = 1000$ points
- Finite difference: $\psi''(i) = \psi(i+1) + \psi(i-1) - 2\psi(i)$
- Strict boundary conditions $\psi(1) = \psi(N_x) = 0$
- Hamiltonian matrix:

$$\begin{aligned} H_{i,i} &= 1 + V(i) \\ H_{i,i\pm1} &= -1/2 \\ H_{i,j} &= 0 \quad \text{otherwise} \end{aligned}$$

- We used Matlab embedded exact diagonalization algorithm

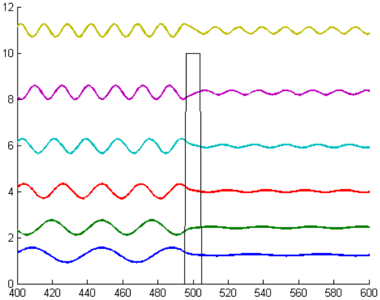
Example of an harmonic potential: $V(x) = \frac{1}{2}\omega^2 x^2$

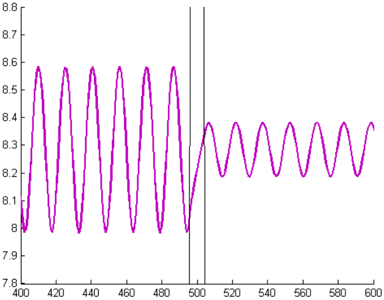




Left: Eigenvectors for an harmonic potential. Right: Comparison of computed eigenvalues (red dots) with the analytical result $E = (n + 1/2)\omega$ (blue line)

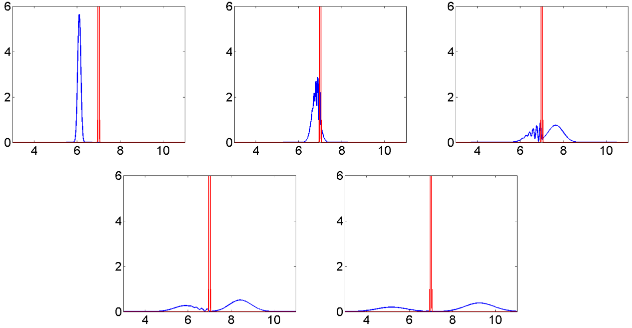
Example of a rectangular potential





Eigenvectors of tunneling problem obtained by the procedure described before with Matlab's exact diagonalization algorithm.

- With the RK4 algorithm
- Discretization: $\Delta x = 5 \cdot 10^{-3}$ and $\Delta t = 2.5 \cdot 10^{-5}$
- The barrier is a very high and narrow gaussian
- Very little loss of norm: about $10^{-5}\%$



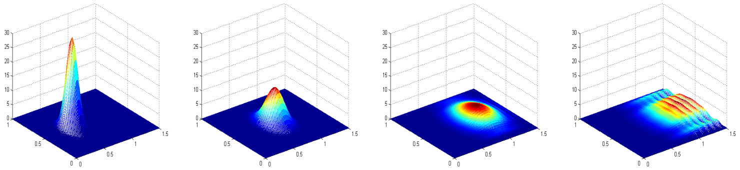
$|\psi(x,t)|^2$ at time steps 1, 950, 2000, 3000 and 4500

Cases in hand of Quantum Mechanics

Bidimensionnal free propagation

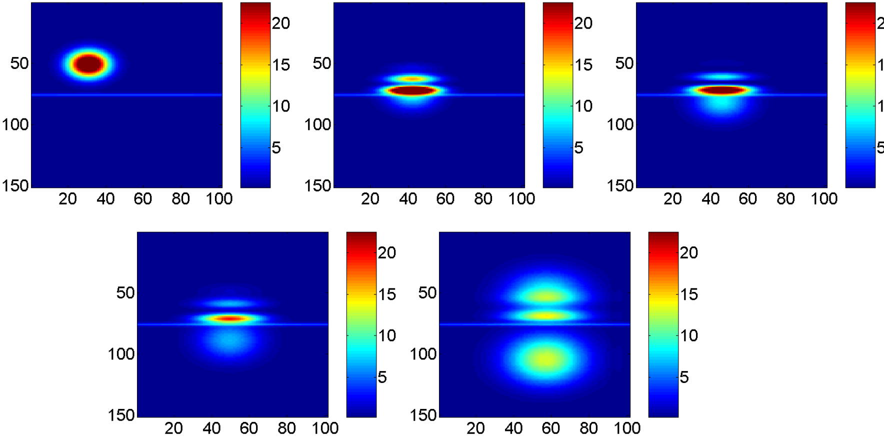
To start, extend the free propagation to two dimensions

- Propagation in the y direction
- Discretization:
  - $\Delta x = 0.025$, 40 points, $\Delta y = 0.005$, 300 points
  - $\Delta t = 2.5 \cdot 10^{-5}$
- Loss of norm: less than 0.02%



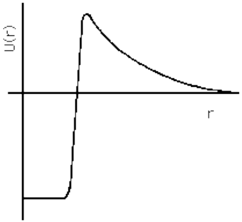
Free propagation and reflexion of a 2D gaussian wave packet. The figures from left to right show the wave packet at time steps 1, 500, 1000 and 1300 when reflexion on boundary infinite walls occurs.

Cases in hand of Quantum Mechanics
Bidimensionnal tunnel effect: Dynamics



$|\psi(x, y, t)|^2$ at time steps 1, 300, 400, 500 and 700

- Effective nuclear potential:



- We observed tunnelling
- Hard to get quantitative results: transmission rate . . .

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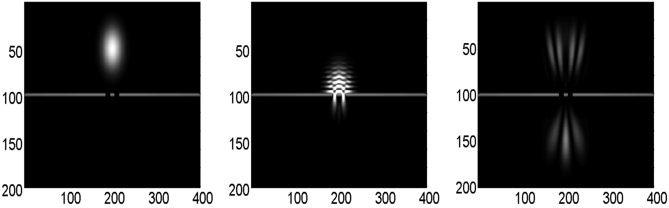
Two slits

- narrow enough so that diffraction occurs
- close enough so that diffracted wave packets interfere



Diffraction of a gaussian wave packet by Young slits. The grey levels represent $|\psi(x, y, t)|^2$. Time steps 1, 1600 and 3680.

- Diffraction appears clearly!
- Interference between two slits also
- However: Hard to check the quantitative validity
  - Not in Fraunhofer conditions: finite distance
  - Gaussian wave packet instead of plane wave ($\Rightarrow$ dispersion e.g.)
- Analytical solution?
  - Hard to derive on our own
  - Not found in articles: more thorough bibliography required!

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Conclusion

- Choice of an accurate and efficient algorithm: RK4
- Quite successful study of some cases in hand of Quantum Mechanics (harmonic potential, 1d and 2d tunnel effect) and comparison with analytical result
- Application to more concrete and complex cases (Gamow model, particle diffraction): qualitatively successful, but hard to interpret quantitatively
- Perspectives:
  - Optimize the code to reach Fraunhofer conditions in the diffraction "experiment"
  - Find an analytical solution for this this case
  - Plenty of other examples of physical interest!

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Thank you for your attention!

Questions?

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