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Numerical Methods in Physics
(5FY033)

Wave packet dynamics.

PURPOSE: To solve the time-dependent Schrödinger equation and study the time evolution of a particle scattering on a square potential.

LITERATURE: Lecture notes

C. M. Dion, A. Hashemloo, and G. Rahali, *Program for quantum wave-packet dynamics with time-dependent potentials*, Comput. Phys. Commun. **185**, 407 (2014).

1 Introduction

The dynamics of a quantum particle are obtained by solving the time-dependent Schrödinger equation. The archetype system is that of a particle scattering on a square potential barrier, which demonstrates many aspects of quantum "weirdness," such as tunneling and above-the-barrier reflexion.

As analytical solutions exist for this problem, it may seem wasteful to study the system numerically. On the other hand, the availability of these solutions offer a great opportunity to test the quality of the simulations.

2 Model

The 1D Hamiltonian to be considered is

$$\hat{H} = \frac{\mathrm{d}^2}{\mathrm{d}^2 x} + V(x), \tag{1}$$

with

$$V(x) = \begin{cases} V_0 & \text{for } u_0 \leq x \leq u_1 \\ 0 & \text{otherwise} \end{cases}. \tag{2}$$

The units are thus chosen such that $\hbar = 1$ and $m = 1/2$, while x will be expressed relative to the length L of the simulation grid (*i.e.*, $0 \leq x \leq 1$). Note that the potential can be negative, *i.e.*, a potential well.

The initial wave function is a Gaussian wave packet following

$$\psi(x; 0) = \left(\frac{1}{\pi \sigma_0^2}\right)^{1/4} \mathrm{e}^{\mathrm{i}k_0 x} \mathrm{e}^{-(x-x_0)^2/2\sigma_0^2}, \tag{3}$$

where k_0 is the initial wave vector, which is related to the average momentum (and hence to the kinetic energy) by $p = \hbar k$. The wave packet should be initially centered at $x_0 = 1/4$ with a spatial width $\sigma_0 = 1/40$.

3 Simulation program

The simulation is to be written using the program WAVEPACKET, which is a general purpose wave-packet-propagation-on-a-grid engine, based on the split-operator method. You will have to write code to implement the model presented in section 2, along with a proper potential and observables, as described in section 4.

The details of the operation of WAVEPACKET can be found in the user manual (see reference on the cover page), in particular section 3.2. To summarize, you need to provide a C source file (including the header `wavepacket.h`) containing the following functions:

- `initialize_potential`
- `potential`
- `initialize_wf`
- `initialize_user_observe` (can be empty)
- `user_observe` (can be empty)

You must also provide a parameter file.

4 Results to produce

4.1 Free evolution

Your first task is to figure out what parameters should be used in the simulation. For this, it is easiest to consider the free evolution of the wave packet, *i.e.*, in the absence of any potential. In this case, starting from the initial condition (3) the analytical solution for the time evolution is

$$\psi(x;t) = \left(\frac{\sigma_0^2}{\pi}\right)^{1/4} \frac{\mathrm{e}^{\mathrm{i}\varphi}}{(\sigma_0^2 + 2\mathrm{i}t)^{1/2}} \mathrm{e}^{\mathrm{i}k_0 x} \exp\left[-\frac{(x - x_0 - 2k_0 t)^2}{2\sigma_0^2 + 4\mathrm{i}t}\right], \tag{4}$$

with

$$\varphi \equiv -\theta - k_0^2 t; \quad \tan 2\theta = 2t/\sigma_0.$$

You should consider values of k_0 in the range $[150, 300]$. *Hint:* the maximum value of k that can be represented on a grid is $k_{\max} = \pi/\Delta x$.

By comparing to the analytical solution, check your numerical results both in terms of the spatial distribution $|\psi(x;t)|^2$ and the complex phase of the wave function. The convergence of the simulation parameters can be checked by reducing the value of Δx and Δt. Halving either of these should not modify the result obtained.

The physical system corresponds to an infinite 1D system, which cannot be represented exactly in the computer with grid methods, which would then require an infinite number of grid points. The effect of truncating the grid to a finite region of space is to modify the physical system at the edge of the grid, and for the simulation to be a good approximation of the real system, the wave packet must never approach the edge of the grid. Study this by actually letting the wave packet travel the entire grid. Describe what happens at the edge of the grid and explain it by considering the particulars of the numerical method you are using.

4.2 Potential well

Consider a potential well with $V_0 = -5 \times 10^4$, and u_0 and u_1 such that the potential is centered on $x = 1/2$ and of width ≈ 0.032 (get as close as possible to this value for the grid spacing Δx you are using). Calculate the transmission and reflection probabilities, as a function of the central momentum of the initial wave packet. These can be obtained by from the integrals

$$R(t) = \int_0^{u_0} |\psi(x;t)|^2 \, \mathrm{d}x \tag{5}$$

and

$$T(t) = \int_{u_1}^{1} |\psi(x;t)|^2 \, \mathrm{d}x, \tag{6}$$

which are here approximated by discrete sums (using the Gauss rule, *i.e.*, multiply by 1/2 the first and last elements of the sum)

You can use the time evolution of these observables to figure out the appropriate length of the simulation. You should also check that the wave packet never reaches either end of the grid and that the parameters of the simulation are converged.

4.3 Square barrier

Repeat the same as the previous section, but with a potential barrier $V_0 = 5 \times 10^4$. Find a case where there is tunneling, *i.e.*, transmission is maximal while the average kinetic energy k_0^2 is less than V_0, and calculate the probability of finding the particle inside the potential barrier. Show how this probability decays with time after the scattering event.

4.4 Bonus exercise

Write a simulation program to study the potential well or the square barrier, but using another numerical algorithm than the split-operator method (see the lecture notes). You need only reproduce one dataset. Choose the wave vector k_0 such that the results are "interesting," based on your previous simulations. Compare the execution time of the two programs.[1]

5 Presentation

Collect your results in a brief report. For the square barrier and potential well simulations, you should present figures showing the time evolution of the wave packet ($|\psi(x;t)|^2$), before, during, and after the scattering event. This in addition to plots

[1] Keep in mind that the split-operator method is well-adapted to time-dependent potentials. It may not fare well against other methods when the potential is static, as is the case here.

presenting observables (*e.g.*, transmission probability) as a function of the momentum of the wave packet. Note that this does not mean that your report should contain too many figures! It is up to you to figure out how to present all of the information you get from the simulations in a concise manner.