Homework problem for the course NTMF058

the year 2022/2023

Note about units: In quantum mechanics, the atomic units are often used, i.e. it is set $\hbar = 1$ a $m_e = 1$. Thus all masses are measured relative to the electron mass. The length unit is Bohr's radius $a_0 \doteq 0{,}529177 \times 10^{-10}$ m. The energy unit is 1 hartree equal to twice the bounding energy of an electron in the ground state of the hydrogen atom, i.e. approximately 27.211 eV. And the time unit $\tau_0 \doteq 2.418884 \times 10^{-17}\,\mathrm{s} \approx 1/40\,\mathrm{fs}$. All equations and numerical values of parameters in these problems are given in atomic units; for simplicity, the atomic units are not explicitly written.

Problem: quantum evolution of one-dimensional systems

Time evolution of the one-dimensional wave function $\psi(x,t)$ in quantum mechanics can be obtained by repeated application of the evolution operator

$$\psi(x, t+\Delta t) = \mathrm{e}^{-iH\Delta t}\psi(x,t)\,, \qquad \psi(x,0) = \psi_0(x)\,, \tag{1}$$

where the Hamiltonian for a particle with mass μ in the potential $V(x)$ has the form

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

Since the computation of the exponential of the operator is not in general simple, various approximations are used, two of which are presented in the subproblems.

In several cases (free particle, harmonic oscillator, eigenstate of the system) the time evolution can be calculated in a closed form. We can thus test programs for time evolution, for example, by acting on a certain eigenstate $\psi_n(x)$ of the system with energy E_n, when the time evolution is given only by a trivial multiplication of the phase factor

$$\psi(x,t) = \mathrm{e}^{-iE_n t}\psi_n(x)\,,$$

where we assume that at time $t = 0$ the system is in its eigenstate $\psi_n(x)$. Or we can use the motion of a free normalized Gaussian wave packet

$$\psi(x, t=0) = (2\pi\sigma^2)^{-1/4}\mathrm{e}^{-(x-x_0)^2/4\sigma^2 + ip_0 x} \tag{3}$$

with the mean position x_0, the mean momentum p_0 and the width σ_0, whose exact time evolution is given by the relations

$$\psi(x,t) = (2\pi\Sigma(t)^2)^{-1/4}\mathrm{e}^{-(x-X(t))^2/4\Sigma(t)^2 + i\phi(x,t)}\,, \tag{4}$$

where

$$\Sigma(t)^2 = \sigma^2 + \frac{t^2}{4\mu^2\sigma^2}\,, \quad X(t) = x_0 + \frac{p_0 t}{\mu}\,,$$

and

$$\phi(x,t) = p_0[x - X(t)] + \frac{p_0^2 t}{2\mu} + \frac{t[x-X(t)]^2}{8\ mu\sigma^2\Sigma(t)^2} + \mathrm{Arg}\left(\frac{1}{\sqrt{\mu + it/(2\sigma^2)}}\right)\,,$$

where $\mathrm{Arg}(z)$ is the function returning the phase of the complex variable z.

1. Write your own program that will solve the time evolution (1) using the Crank-Nicolson method, where the evolution operator is approximated by the Padé approximant [1/1]

$$\mathrm{e}^{-iH\Delta t} \approx \frac{1 - iH\Delta t/2}{1 + iH\Delta t/2}\,.$$

At the same time, express the wave functions and the Hamiltonian on a uniform grid $x_i = x_0 + ih$ for $i = 0, \ldots, n$, while x_0, h and n must be appropriately chosen for the given task so that throughout the time evolution, it was possible to assume that $\psi(x_0) = \psi(x_n) = 0$. Approximate the second derivative using the basic finite-difference formula

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} \approx \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{h^2}\,,$$

making the $1 \pm iH\Delta t/2$ operators tridiaginal matrices with the potential $V(x)$ added to the main diagonal. The solution of the one timestep then takes place in two steps, first, we multiply the wave function by the tridiagonal matrix

$$z(x) = (1 - iH\Delta t/2)\psi(x,t)$$

and then we solve a system of linear equations with the tridiagonal matrix corresponding to the equation

$$(1 + iH\Delta t/2)\psi(x, t + \Delta t) = z(x)\,.$$

Test the method on the above analytically solvable cases. Verify that the error behaves as Δt^2 in time. Then apply it to the motion of the Gaussian wavepacket (3) in the field of the linear harmonic oscillator $V(x) = \mu\omega^2 x^2/2$. Determine the period (i.e. the distance between the maxima of the autocorrelation function $c(t) = \langle\psi(t)|\psi(0)\rangle$) of its motion in the potential for a specific choice of parameters $\mu = 1$, $\omega = 1.5$, $x_0 = -5$, $p_0 = 0$ and $\sigma = 0.5$. What parameters does this period depend on? Does the obtained value correspond to the classical period?

2. Write your own program that will solve time evolution (1) using the split-operator method, where the evolution operator is approximated by

$$\mathrm{e}^{-iH\Delta t} \approx \mathrm{e}^{-iV\Delta t/2}\mathrm{e}^{ip^2\Delta t/2m}\mathrm{e}^{-iV\Delta t/2}\,.$$

Express the wave function on a uniform grid $x_i = x_0 + ih$ for $i = 0, \ldots, n$, where x_0, h and n must be appropriately chosen for the problem so that throughout the whole time evolution, it is possible to assume that $\psi(x_0) = \psi(x_n) = 0$. Choose the number of points so that $n - 1 = 2^k$ for efficient use of the fast Fourier transform, which is used to go to the p representation after applying to $\psi(x,t)$ the operator $\mathrm{e}^{-iV\Delta t/2}$ (multiplication by the numbers $\mathrm{e}^{-iV(x_i)\Delta t/2}$), thereby reducing the action of the operator $\mathrm{e}^{ip^2\Delta t/2m}$ again to multiplication, this time in p-space. Then go to the x-space again with the inverse transform and repeat the process. In this task, you do not need to code the FFT method, but you can use one of the libraries to calculate it.

Test the method on the above analytically solvable cases. Verify that the error behaves as Δt^2 in time. Then apply it to the motion of the Gaussian wavepacket (3) in the field of the linear harmonic oscillator $V(x) = \mu\omega^2 x^2/2$. Determine the period (i.e. the distance between the maxima of the autocorrelation function $c(t) = \langle\psi(t)|\psi(0)\rangle$) of its motion

in the potential for a specific choice of parameters $\mu = 1$, $\omega = 1.5$, $x_0 = -5$, $p_0 = 0$ and $\sigma = 0.5$. What parameters does this period depend on? Does the obtained value correspond to the classical period?