Computational Physics – Exam exercise

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Quantum harmonic oscillator

- Solve the time-dependent Schrödinger equation for the 1-dimensional harmonic oscillator

$$i\frac{\partial}{\partial t}\Phi(x,t)=\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{\Omega^2}{2}x^2\right)\Phi(x,t)$$

  - Note: all variables are dimensionless ($\hbar = m = 1$)
- Use the second-order product formula

$$e^{-i\tau H} \approx e^{-i\tau K_1/2}e^{-i\tau K_2/2}e^{-i\tau V}e^{-i\tau K_2/2}e^{-i\tau K_1/2}$$

Things to show

- Plot $P(x,t)\mathrm{dx} = |\Phi^*(x,t)\Phi(x,t)|\mathrm{dx}$ for t=0,2,…,10
- Compute

$$\langle x(t)\rangle = \int_{-\infty}^{+\infty} x\,|\,\Phi^*(x,t)\Phi(x,t)\,|\,dx$$

$$\langle x^2(t)\rangle = \int_{-\infty}^{+\infty} x^2\,|\,\Phi^*(x,t)\Phi(x,t)\,|\,dx$$

- Plot $\langle x(t)\rangle$ and $\langle x^2(t)\rangle - \langle x(t)\rangle^2$ for t=0,…,10 (e.g. in steps of 0.1)

Parameters etc.

- Discretize the problem as explained in the course

$$-15 \le x \le 15, \quad \Delta = 0.025 \quad , \quad L = 1001 \quad , \quad \tau = 0.00025 \quad , \quad m = 40000$$

- Initial wave packet

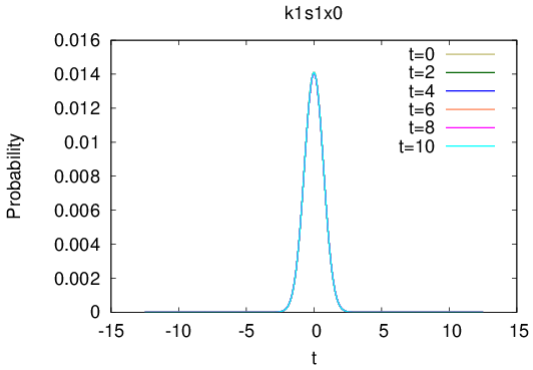
$$\Phi(x, t=0) = (\pi\sigma^2)^{-1/4} e^{-(x-x_0)^2/2\sigma^2}$$

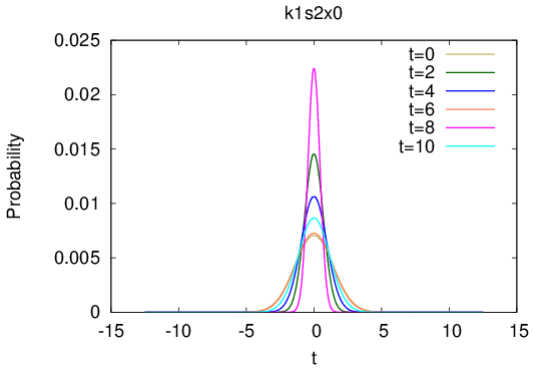
- Show cases

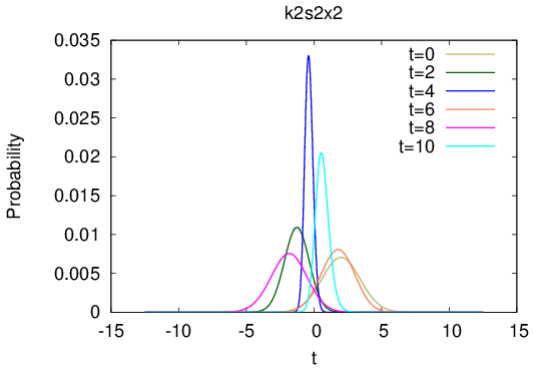
$$(\Omega, \sigma, x_0) = (1,1,0), (1,1,1), (1,2,0), (2,1,1), (2,2,2)$$

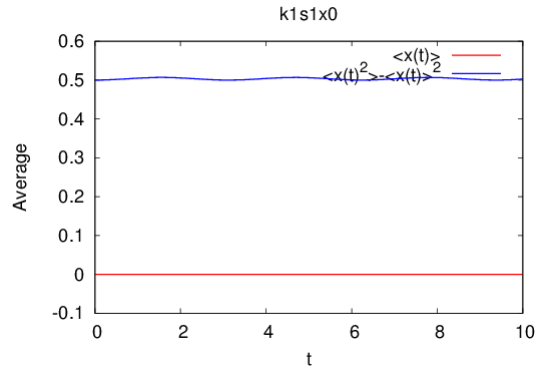
- Find the analytical expression for $\langle x(t) \rangle$ and $\langle x^2(t) \rangle - \langle x(t) \rangle^2$ and give a qualitative discussion/interpretation of the simulation results
  - Hint: set $x_0 = 0$ for simplicity and then extend to the general case

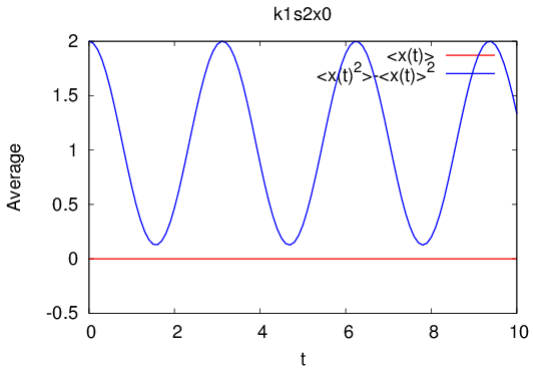
Some examples

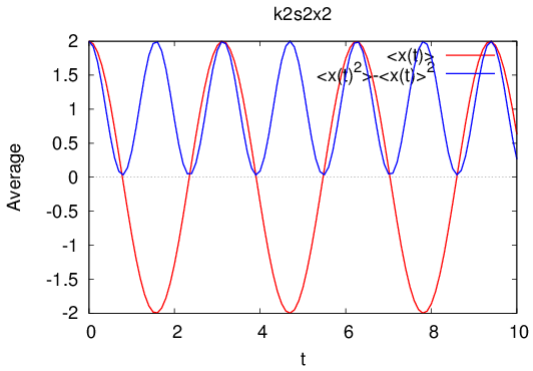












Note

- The values for the parameters for the discretization in space and time are indicative
  → they do not have to be considered to be "strict" values
  → you are allowed to take other values if you think they result in better results/figures

Work out the solutions and write a report on your own (forming working groups of 2 persons is not allowed for the exam)

Report

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- Filename: Exam_Surname.pdf
- Content of the report:
  - Name + matricle numbers+ e-mail address + title
  - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
  - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
  - Simulation results: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
  - Discussion: summarize your findings
  - Appendix: Include the listing of the program

Due date: 10 AM, July 28, 2023 (**STRICT**)

Marks

- Correct program and nice figures: 50%
- Good introduction describing the problem and simulation method: 25%
- Analytical work + interpretation of the results : 25%