PC4230 Project, Semester I, AY 2024-2025, **due date: November 29, 2024**
(totally 3 pages)

Instructions.

1. **Objective**: This project is mainly (i) to train you to develop more proficiency in applying Matlab to quantum mechanics problems, especially to the simulation of quantum dynamics, and (ii) to have more experiences in critically analyzing computational results in connection with theoretical insights.

2. **Work mode**: You may find one partner from this class to team up or work on this individually. Other than the expected collaboration within a team, you are not allowed to discuss among yourselves about specific aspects of the project execution. However, if you are not clear about any basic concepts (e.g., DVR, FFT, Split-operator method), you may still consult your classmates or the lecturer.

3. **Consultation sessions:** Along the way, you are expected to contact the lecturer to discuss difficulties you have met or the progresses you have made. We will set aside one lecture slot (2-4 pm, 19th September, Thursday) for everybody to discuss with lecturer and clarify your questions about this project (so no new materials on that day). After this, you are still encouraged to arrange additional consultation sessions with the lecturer.

4. **Deliverable**: Please submit a printout of your Matlab code, together with a report with necessary graphs, discussions and interpretations of your results (e.g., how you choose your parameters, how you compare theory with "numerical experiments", how you implement your codes, what you view as particularly interesting, why do you think you have observed multi-photon transitions etc). Ideally, your report should be clearly structured and easily readable.

Working Project:

Consider a particle moving in a harmonic oscillator potential, with the associated dimensionless Hamiltonian given by

$$H^0 = \frac{p^2}{2} + \frac{1}{2}x^2$$

with the effective $\hbar = 1$. In terms of the dimensionless units adopted here, the energy level spacing is 1.0 and initially the system is in its ground state. We now switch on a time-periodic perturbation $V(t)$ (t is in dimensionless units here), whose dimensionless form is given by $V(t) = A\sin(x)\cos(\omega t)$, with A being the driving amplitude and ω the driving frequency. To examine the ensuing dynamics you are now asked to adapt the code you learned before to implement the split-operator method for time-dependent Hamiltonians. To that end you need to divide the time into many small intervals, and within each small time window, you can still approximate the Hamiltonian as a constant and then use the split-operator method to obtain the evolution operator for each small time interval.

1. Please adapt the circulated codes on Canvas to simulate the time evolution of this system. Before you do any physical investigations, make sure that your results have convergence (that is, physics observed is no longer dependent on time step size, number of DVR points etc). Make interesting observations by tuning A and ω.

2. You may use analytical forms of the eigenstates of a harmonic oscillator available from internet (note that Hermite polynomials can be directly called in Matlab) when you need to define the initial state or when you analyze the quantum amplitude projected onto the eigenstates of the unperturbed Harmonic oscillator system. You may also numerically generate the ground state and all other excited states from the DVR approach we studied. For the second approach, some caution is needed as the convention (and boundary conditions) in our lectures for defining the grid points used in DVR for spectrum calculations and that for FFT calculations are slightly different and so you need to do something about it.

3. Please analyze the transition probabilities from the ground state to the first excited state when the driving frequency is almost on-resonance with the natural frequency of the harmonic oscillator. In particular, how does the transition probability depend on time and on the driving frequency? You are encouraged to discuss any feature that is

interesting to you. Remember, you are actually doing an experiment and so feel free to explore.

4. Compare your results from step 3 with our first-order time-dependent perturbation theory with or without the so-called rotating-wave approximation. Analyze how first-order time-dependent perturbation theory breaks down as A increases.

5. As we increase the driving field amplitude A, is there any two-photon transition probability from the ground state to the first excited state if $\omega \approx 0.5$? That is, are the transitions from the ground state to the first excited state due to off-resonance one-photon processes or due to any two-photon processes? What is your reasoning?

6. Consider now $\omega \approx 2.0$, which is almost equal to the transition frequency between the ground state and the second excited state. What would the first-order perturbation theory predict regarding the transition probabilities from the ground state to the second excited state? What do you see from your numerical simulations? What about the transition probabilities to the fourth excited state when $\omega \approx 2.0$ – How to explain your simulation results in terms of some theory we studied already?

7. (**More adventure**). You are encouraged to go beyond what is assigned above (e.g., introducing nonlinearities to the oscillator, considering multiple driving fields, and considering a very small driving frequency etc). Remember, what you have now is basically a small computational lab and how much you can "discover" is mainly limited by how much you are willing to try.