Quantum Mechanics 3 - Homework 1

due date: 10.11.2022

1. In class we found analytically the transition probability for a two-state system, using the rotating wave approximation. In this exercise, you will solve for the transition probability numerically! Write a program[1] (Matlab is recommended, but other programs are fine) that computes the transition probability $P_{1\to 2}(t)$. At the end of the calculation, your program should generate a single graph of the transition probability as a function of time. Compare your result with the analytical result we obtained in class and explain any differences. Attach the graph and a PDF page of your code to the solution.

   Guidance:

   - Work with the same Hamiltonian we used in class, $\hat{H}(t) = \frac{E}{2}\hat{\sigma}_z + \epsilon\cos(\omega t)\hat{\sigma}_x$.
   - Set the initial state at $|\psi(t_0 = 0)\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ and evolve the state according to

     $$|\psi(t_{n+1})\rangle = \exp\left[-i\hat{H}(t_n)\Delta t/\hbar\right]|\psi(t_n)\rangle, \tag{1}$$

     where $\Delta t = t_{n+1} - t_n$ is the difference between adjacent time samples.
   - Stop the evolution at $t_N = 1$. How many time samples N are required to achieve accurate results?
   - Work in units where $\hbar = 1$. Set $\epsilon = 4\pi$, $\omega = 50$, $\delta = 0.01\epsilon/\hbar$. **Bonus:** What is the maximal value of δ for which the rotating wave approximation still holds?

[1] If you don't know, you are required to look up in the web how to construct vectors, matrices, set of matrices, loops and more.

2. An instant electric field $\vec{E}(t,\vec{r}) = A\delta(t)\hat{r}$ ($\hat{r}$ is the unit vector in the radial direction) acts on a hydrogen atom. Find the transition probability from the ground state to the first excited state after the field is turned off, by following the steps below:

   (a) What is the potential $V(t)$ which is associated with $\vec{E}$?

   (b) Using Eq. (1.80) from the lecture notes, obtain an expression for $\hat{U}(t,t_0)$ (the full evolution operator) in the form of an integral. This integral should depend on $\hat{U}_0(t,t_0)$ (the evolution operator that corresponds only to the hydrogen atom part in the Hamiltonian), $\hat{V}(t)$ and $\hat{U}(t,t_0)$ itself.

   (c) Plug $V(t)$ from (a) and solve the integral to find $\hat{U}(0,t_0)$.

   (d) Use the last result to find a close expression for $\hat{U}(t,t_0)$. This expression should depend only on $\hat{U}_0(t,t_0)$ and $\hat{r}$.

   (e) The ground state of the hydrogen atom is $|100\rangle$, while the first excited state is $|2\ell m\rangle$. Which values of ℓ and m don't give zero transition probability? (think physically here)

   (f) Now, take the limit $t_0 \to 0$, and use the relations between $\hat{U}_0(t,t_0)$ and the eigen-states of the hydrogen atom to calculate the transition probability. The answer should be in the form of an integral over r and depend on A. Calculate the integral NUMERICALLY as function of A and plot the result. What is the value of A for which the transition probability is maximal?

   (g) Assume that A is "small enough" and calculate ANALYTICALLY the integral over r from the previous item by taking the leading order in A.

3. Harmonic oscillator is in the ground state at $t \to -\infty$. A time-dependent force $F(t)$ is applied and the corresponding Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega \hat{x}^2 - \hat{x} F(t) . \tag{2}$$

What is the probability that the oscillator ends up in the n'th state when $t \to \infty$, in terms of the force $F(t)$?

Guidance:

- Recall that the n'th state of the harmonic oscillator is given by $|n\rangle = \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}} |0\rangle$, where $\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$ is the ladder operator. Thus, the probability in question should depend on $\hat{a}^\dagger (t \to \infty)$.
- Express the Hamiltonian in terms of the ladder operators $\hat{a}$ and $\hat{a}^\dagger$ and use Heisenberg's equation to find a differential equation for $\hat{a}^\dagger (t)$.
- Assume that $F(t \to \pm\infty) \to 0$ and find the appropriate boundary condition for the differential equation.
- Solve the differential equation and find $\hat{a}^\dagger (t \to \infty)$. Your answer should be in the form of an integral over $F(t)$. Call this integral B.
- Finally, find the transition probability in terms of B. Use here the binomial formula to simplify the answer.