0.1 Time dependence

Rotor

A particle is moving on a circle. The corresponding wavefunctions have the form of $\psi_n = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{i\phi n}$, where $n \in Z$ are the angular quantum numbers. The eigenenergies are $\epsilon_n = \frac{n^2\hbar^2}{2I}$, where I is the moment of inertia.

- Find the time dependent expectation value of the momentum operator $p = -i\hbar\frac{d}{d\phi}$ for a state n.
- Find the time dependent expectation value of the x component of the position operator for a state n. Assume that $x = cos(\phi)$.

Now suppose that the particle is in a state equally composed by the ground state and first excited state $\psi = N(\psi_0 + \psi_1)$.

- What are the time dependent expectation values of the momentum and position operators for this state?

Particle in a square well potential

A particle is moving in an infinitely deep square well potential on an interval $(0, a)$. The wavefunction is equally composed by the two lowest lying states $\psi = N(\psi_1 + \psi_2)$.

- Find the value of the normalisation constant N.
- Find the expectation value of the position operator x for $t = 0$.
- Write down the wavefunction including the time dependence.
- Find the expectation value of the position operator x including the time dependence, i.e. $\langle x\rangle(t)$.
- What would be the time dependent expectation value for wavefunction of the form $\psi = N(\psi_1 + \psi_3)$?

Hint: The wavefunctions for the particle are

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\,.$$

The general solution of the time dependent Schrödinger equation is

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \mathrm{e}^{-i\epsilon_n t/\hbar}\psi_n(x)\,.$$

Two state system

An effective Hamiltonian of a system has two levels, $|a\rangle$ and $|b\rangle$ with eigenenergies ϵ_a and ϵ_b. An operator $\hat{A}$ has two eigenvectors that correspond to $|A_1\rangle = \frac{1}{\sqrt{2}}(|a\rangle + |b\rangle)$ and $|A_1\rangle = \frac{1}{\sqrt{2}}(|a\rangle - |b\rangle)$, with eigenvalues a_1 and a_2, respectively.

- What are the expectation values of the energies of the system for the states $|A_1\rangle$ and $|A_2\rangle$?
- What is the matrix representation of the operator $\hat{A}$ in the basis of the eigenvectors of the Hamiltonian? *Hint: operator can be written as* $A = \sum_i |i\rangle a_i \langle i|$, *where* a_i *are the eigenvalues and* $|i\rangle$ *are the corresponding eigenvectors.*
- What are the expectation values of the operator A for the eigenstates $|a\rangle$ and $|b\rangle$?
- Show that you obtain the correct eigenvalues of the operator A by diagonalising its matrix representation.
- Write down the time dependent wavefunctions of states $|A_1\rangle$ and $|A_2\rangle$, using the eigenstates of the Hamiltonian.
- What is the time dependent expectation value of the operator A if at time $t = 0$ the system was found to be in the state $|A_1\rangle$?

Evolution in imaginary time

At time zero the wavefunction of a system is composed of any combination of the eigenfunctions and includes the ground state wavefunction. That is $\Psi(t = 0) = \sum_{i=0}^{\infty} \psi_i$. The system is then evolved in imaginary time τ. Show that for $\tau \to \infty$ only the ground state will be present in the wavefunction.

Note: The evolution in imaginary time is used in the diffusion Monte Carlo method (QMC). QMC is one of the few techniques that can be applied to obtain accurate quantum mechanical energies of systems with a large number of atoms.