Exam Quantum Dynamics, NWI-SM295

Prof. dr. ir. Gerrit C. Groenenboom, HG03.054, 14:00-17:00, July 21, 2014

Question 1: Flux

The Hamiltonian for a particle with mass m moving in a one dimensional potential $V(x)$ is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

A time dependent wave function $\psi(x,t)$ satisfies the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t).$$

1a. Give an expression for the probability $P_{ab}(t)$ that the particle is in the interval $a < x < b$ at time t.

1b. Give the relation between the flux j_a at $x = a$, the flux j_b at $x = b$ and the time derivative of the probability $dP_{ab}(t)/dt$.

1c. Derive the general expression for the flux j_x of wave function $\psi(x,t)$.

Question 2: The interaction picture

The so called "interaction picture" can simplify the solution of the time-dependent Schrödinger equation, in particular when the Hamiltonian consists of a time-independent part $\hat{H}_0$ and a time-dependent part $\hat{V}(t)$:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t).$$

The solution of the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(t) = \hat{H}(t)\Psi(t)$$

is written as

$$\Psi(t) = e^{-\frac{i}{\hbar}\hat{H}_0 t}\Psi_I(t).$$

The function $\Psi_I(t)$ is called "the wave function in the interaction picture". It satisfies an equation that is very similar to the Schrödinger equation:

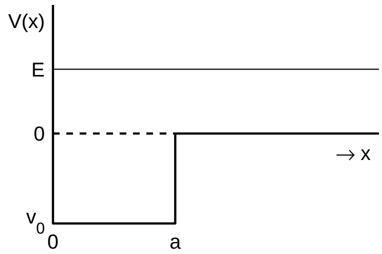
$$i\hbar \frac{\partial}{\partial t}\Psi_I(t) = \hat{A}(t)\Psi_I(t).$$

2a. For given $\hat{H}_0$ and $\hat{V}(t)$, derive an expression for $\hat{A}(t)$ and simplify it as much as possible. Keep in mind that $\hat{H}_0$ and $\hat{V}(t)$ may not commute.

2b. Is $\hat{A}(t)$ Hermitian? Derive your answer, assuming that $\hat{H}_0$ and $\hat{V}(t)$ are Hermitian.

2c. What is the physical meaning of $\Psi_I(t)$ when the Hamiltonian $\hat{H}$ is time-independent, i.e., when $\hat{V}(t) = 0$?

Question 3: Scattering for one-dimensional square well



The Hamiltonian for a one-dimensional square well potential is given by

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x),$$

where μ is the mass of the particle. The square-well potential is given by

$$V(x) = \begin{cases} +\infty & \text{for } x \leq 0, \\ v_0 & \text{for } 0 < x < \text{a}, \\ 0 & \text{for } x > a, \end{cases}$$

as shown by the thick line in the figure.

The K-matrix boundary conditions for time-independent scattering are

$$\Psi(x) = \begin{cases} 0 & \text{for } x = 0, \\ \sin(kx) + K\cos(kx) & \text{for } x > a, \end{cases}$$

where k is the magnitude of the wave vector.

3a. Sove the K-matrix for arbitrary E, μ, a, and v_0.

3b. What are the S-matrix boundary conditions for this problem?

3c. Give the expression for the S-matrix as function of the K-matrix.

Question 4: Matrix representations of rotations

In two dimensions a rotation over an angle ϕ is represented by a 2×2 matrix, that can be written in exponential form as

$$\boldsymbol{R}(\phi) = e^{\phi \boldsymbol{N}}$$

where

$$\boldsymbol{N} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

4a. Compute the matrix $\boldsymbol{R}$ by evaluating the exponential (*hint:* $\boldsymbol{N} = i\boldsymbol{H}$, *where* $\boldsymbol{H}$ *is Hermitian. Use the eigenvalues and eigenvectors of* $\boldsymbol{H}$.).

The general expression for a three-dimensional rotation operator in angular momentum space, in atomic units, is given by

$$\hat{R}(\boldsymbol{n}, \phi) = e^{-i\phi \boldsymbol{n}\cdot\hat{\boldsymbol{j}}}, \qquad (1)$$

where ϕ is the angle, $\boldsymbol{n}$ is a vector with $|\boldsymbol{n}| = 1$, and $\hat{\boldsymbol{j}}$ is the angular momentum operator. The representation of $\hat{R}(\boldsymbol{n}, \phi)$ in the $2j+1$ dimensional angular momentum space $\{|jm\rangle, m = -j, -j+1, \ldots, j\}$ is defined by

$$\hat{R}(\boldsymbol{n}, \phi)|jk\rangle \equiv \sum_m |jm\rangle D^j_{m,k}(\boldsymbol{n}, \phi). \qquad (2)$$

4b. Derive an expression for all matrix elements $D^j_{m,k}(\boldsymbol{e}_z, \phi)$,

where

$$\boldsymbol{e}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Let

$$\hat{R}(\boldsymbol{n}_1, \phi_1) = \hat{R}(\boldsymbol{n}_2, \phi_2)\hat{R}(\boldsymbol{n}_3, \phi_3).$$

4c. Use Eq. (2) to prove the matrix-representation property

$$\boldsymbol{D}^j(\boldsymbol{n}_1, \phi_1) = \boldsymbol{D}^j(\boldsymbol{n}_2, \phi_2)\boldsymbol{D}^j(\boldsymbol{n}_3, \phi_3).$$

4d. Show, starting with Eqs. (1) and (2), that

$$\boldsymbol{D}^j(\boldsymbol{e}_y, \phi) = e^{-i\phi \boldsymbol{J}_y},$$

where $\boldsymbol{J}_y$ is the matrix representation of $\hat{j}_y$.