Chapter 2: Quantum Dynamics in Hilbert Space

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1 Overview

Chapter 2 introduces the reader to the Time-Dependent Schrödinger equation (TDSE) and defines the time propagator operator ($U(t, t_0)$). The two level system is provided as an example of solving the TDSE and the corresponding time propagator operator is determined. The interaction picture is used to simplify the problem from the Schrödinger picture and various properties are shown. Lastly, the Greens function within the frequency domain is used to model the proposed Wigner and Weisskopy of irreversible decay.

2 Time-Evolution Operator with Time-Dependent Hamiltonian

Within the Schrödinger picture, the TD wavefunction in the position space $\mathbf{x}$ is given by

$$\psi(\mathbf{x}, t) = \langle \mathbf{x} | \psi(t) \rangle \tag{1}$$

and the TDSE will be defined as

$$\frac{\partial |\psi(t)\rangle}{\partial t} = -\frac{i}{\hbar} H |\psi(t)\rangle \tag{2}$$

and solutions to Eqn (2) are the eigenvectors $|\phi_n(t)\rangle$ with corresponding eigenvalues E_n. These eigenvections form a complete basis set and satisfy the completness condition $\sum_n |\phi_n\rangle\langle\phi_n| = 1$. We can expand the wavefunction $\psi(t)$ within this basis,

$$|\psi(t)\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi(t)\rangle. \tag{3}$$

Substitution of Eqn (3) into the TDSE yields

$$\frac{d}{dt}\langle\phi_n|\psi(t)\rangle = -\frac{i}{\hbar} E_n \langle\phi_n|\psi(t)\rangle, \tag{4}$$

which is 1st-order differential equation with the solution

$$\langle\phi_n|\psi(t)\rangle = \sum_n e^{-\frac{iE_n}{\hbar}(t-t_0)} |\phi_n\rangle\langle\phi_n|\psi(t_0)\rangle. \tag{5}$$

The general time evolution operator is defined as

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle. \tag{6}$$

A few properties of the time evolution operator are that $U(t_0, t_0) = 1$ and unitary $U^\dagger U = 1$. The usefulness of this operator provides the means to solve the time evolution of the system in general without needing specific initial conditions. Hence, the TDSE only needs to be solved once with the corresponding $U(t, t_0)$ which may operate on any intial state $|\psi(t_0)\rangle$. Based on Eqn (5) and (6), the time evolution operator is

$$U(t, t_0) = \sum_n |\phi_n\rangle e^{-\frac{iE_n}{\hbar}(t-t_0)} \langle\phi_n|. \tag{7}$$

The current form of $U(t,t_0)$ is limited to the representation of the Hamiltnian H and a general form is provided for greater flexibility. This will allow semiclassical approximations. The general form can be obtained by the concept of a function of an operator via Taylor series expansion. Given function $f(A)$ for operator A, the Taylor series can be seen as

$$f(A) \equiv \sum_{p=0}^{\infty} \frac{f^{(p)}(0)}{p!} x^p \tag{8}$$

$$f(A) = \sum_{p=0}^{\infty} \frac{f^{(p)}(0)}{p!} x^p \equiv f(a_j)|\alpha_j\rangle\langle\alpha_j \tag{9}$$

With Eqns (7) and (9), the $U(t,t_0)$ is recasted into the form

$$U(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}. \tag{10}$$

2.1 Two-level System Example

Section 2 reviews the TD quantum mechanic equations and introduces the generalized time evolution operator. With the tools, an example of the time evolution operator is demonstrated for a coupled two-level system ($|\phi_a\rangle$ and $|\phi_b\rangle$), with energies ϵ_a and ϵ_b, and a coupling V_{ab}, represented by the Hamiltonian

$$H = \begin{pmatrix} \epsilon_a & V_{ab} \\ V_{ba} & \epsilon_b \end{pmatrix} \tag{11}$$

where $V_{ab} - V*_{ba} = |V_{ab}|E^{-i\chi}$, $0 < \chi < 2\pi$. This can be made into an eigenvalue problem

$$H \begin{pmatrix} |\phi_a\rangle \\ |\phi_b\rangle \end{pmatrix} = \begin{pmatrix} \epsilon_a & V_{ab} \\ V_{ba} & \epsilon_b \end{pmatrix} \begin{pmatrix} |\phi_a\rangle \\ |\phi_b\rangle \end{pmatrix} = \epsilon_{\pm} \begin{pmatrix} |\phi_a\rangle \\ |\phi_b\rangle \end{pmatrix} \tag{12}$$

Diagonalize the Hamiltonian,

$$\det(H - \lambda\mathbf{1}) = 0 \tag{13}$$

$$(\epsilon_a - \lambda)(\epsilon_b - \lambda) - |V_{ab}|^2 = 0 \tag{14}$$

$$\lambda^2 - \lambda(\epsilon_a + \epsilon_b) + \epsilon_a\epsilon_b - |V_{ab}|^2 = 0 \tag{15}$$

$$\lambda = \frac{(\epsilon_a + \epsilon_b) \pm \sqrt{(\epsilon_a + \epsilon_b)^2 - 4\epsilon_a\epsilon_b + 4|V_{ab}|^2}}{2} \tag{16}$$

$$= \frac{(\epsilon_a + \epsilon_b) \pm \sqrt{(\epsilon_a - \epsilon_b)^2 + 4|V_{ab}|^2}}{2} \tag{17}$$

Eigenvectors corresponding to eigenvalues λ are

$$\begin{pmatrix} \frac{\epsilon_a - \epsilon_b \pm \sqrt{(\epsilon_a - \epsilon_b)^2 + 4|V_{ab}|^2}}{2V} & 1 \end{pmatrix} \tag{18}$$

The corresponding generalized eigenvectors ($|\psi_{\pm}\rangle$) are simply linear compinations of $|\phi_a\rangle$ and $|\phi_b\rangle$ with the associated radiation phase $e^{\pm i\chi}$. These are rotated eigenvectors from Eqn (18)

$$\begin{pmatrix} |\psi_+\rangle \\ |\psi_-\rangle \end{pmatrix} = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} e^{-i\chi/2}|\phi_a\rangle \\ e^{i\chi/2}|\phi_b\rangle \end{pmatrix} = \begin{pmatrix} \cos(\theta)e^{-i\chi}|\phi_a\rangle + \sin(\theta)e^{i\chi}|\phi_b\rangle \\ \cos(\theta)e^{-i\chi}|\phi_a\rangle - \sin(\theta)e^{i\chi}|\phi_b\rangle \end{pmatrix} \tag{19}$$

θ is a transformation angle that can be determined with Eqns (18) and (19). The work is shown in the mathematica notebook

$$\tan 2\theta \equiv \frac{2|V_{ab}|}{\epsilon_a - \epsilon_b},\ 0 < \theta < \pi/2 \tag{20}$$

Within this basis, the time evolution operator is given by

$$U(t,t_0) = |\psi_+\rangle e^{-\frac{i\lambda_+}{\hbar}(t-t_0)}\langle\psi_+| + |\psi_-\rangle e^{-\frac{i\lambda_-}{\hbar}(t-t_0)}\langle\psi_-| \tag{21}$$

2.2 Progating the two-level system

Suppose the system is at initial time $t_0 = 0$ in the $|\phi_a\rangle$ state and the probability that the system is in $|\phi_b\rangle$ at time t.

$$P_{ab}(t) \equiv |\langle\phi_b|\psi(t)\rangle|^2 = |\langle\phi_b|U(t,t_0)|\phi_a\rangle|^2 \tag{22}$$

The states $|\phi_a\rangle$ and $|\phi_b\rangle$ are defined as unit vectors and the substitution of Eqn (21) into Eqn (22) will yield the probability to be in state $|\phi_b\rangle$ at a given time t. From mathematica, the $P_{ab}(t)$ is given as

$$P_{ab}(t) = \sin^2(2\theta)\sin^2\left(\frac{\lambda_- - \lambda_+}{2\hbar}t\right) \tag{23}$$

$$= \frac{4|V_{ab}|^2}{4|V_{ab}|^2 + (\epsilon_a - \epsilon_b)^2}\sin^2\left(\sqrt{4|V_{ab}| + (\epsilon_a - \epsilon_b)^2}\frac{t}{2\hbar}\right) \tag{24}$$

The step from Eqn (23) to (24) is using Eqn (20), the trignometry identity $\sin^2 2\theta + \cos^2 2\theta = 1$, and substituting in the eigenvalues λ. This is left for the reader to derive. Figure 1 is the plot of the probability for various coupling constants V_{ab}. This is known as the Rabi formula and

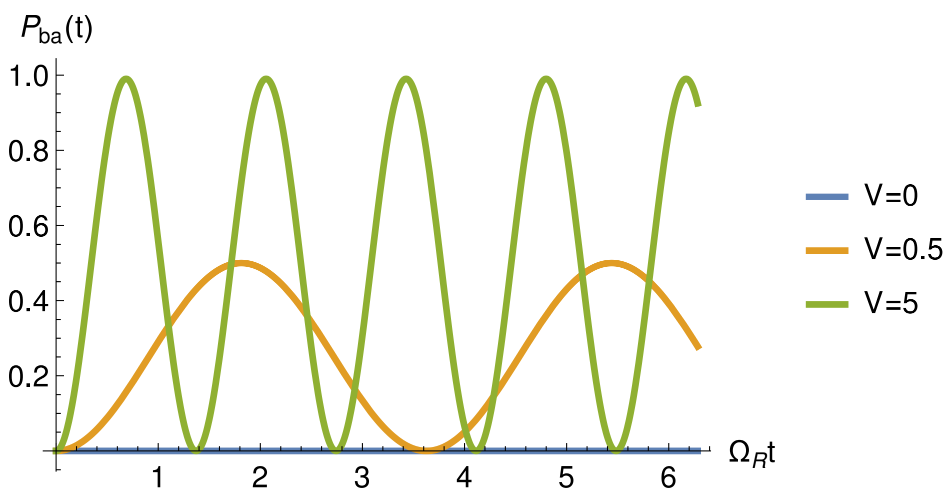

Figure 1: Rabi oscillation of the two level system for coupling constant V_{ab} at 0, 0.5, and 5.

$$\Omega_{\mathrm{R}} = \sqrt{4|V_{ab}| + (\epsilon_a - \epsilon_b)^2}/\hbar \tag{25}$$

is the Rabi frequency.