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}.

$$\begin{aligned}
\left(\tan 2\theta = \frac{2|V_{ab}|}{\epsilon_a - \epsilon_b}\right)^2 \\
\tan^2(2\theta) &= \frac{4|V_{ab}|^2}{(\epsilon_a - \epsilon_b)^2} \\
\sin^2(2\theta) + \cos^2(2\theta) &= 1 \\
\tan^2(2\theta) &= \frac{1}{\cos^2(2\theta)} - 1 \\
&= \frac{4|V_{ab}|^2}{(\epsilon_a - \epsilon_b)^2} \\
\frac{1}{\cos^2(2\theta)} &= \frac{4|V_{ab}|^2 + (\epsilon_a - \epsilon_b)^2}{(\epsilon_a - \epsilon_b)^2} \\
\cos^2(2\theta) &= \frac{(\epsilon_a - \epsilon_b)^2}{4|V_{ab}|^2 + (\epsilon_a - \epsilon_b)^2} \\
&= 1 - \sin^2(2\theta) \\
\sin^2(2\theta) &= \frac{4|V_{ab}|}{4|V_{ab}|^2 + (\epsilon_a - \epsilon_b)^2}
\end{aligned}$$

This is known as the Rabi formula and

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

is the Rabi frequency.

2.3 Propagation with Time-Dependent Hamiltonians: Time Ordering

The generalize definition of the time-evolution operator to the time-dependent Hamiltonian,

$$\frac{\partial}{\partial t}U(t,t_0)|\psi(t_0)\rangle = -\frac{i}{\hbar}H(t)U(t,t_0)|\psi(t_0)\rangle. \tag{26}$$

Upon integration, the time propagator operator is

$$U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H(t)U(t,t_0). \tag{27}$$

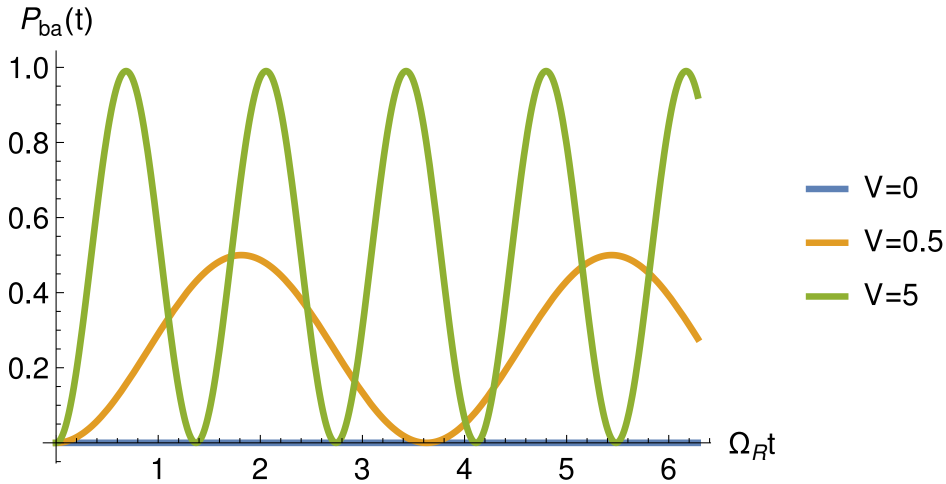

Figure 1: Rabi oscillation of the two level system for coupling constant V_{ab} at 0, 0.5, and 5.

Eqn (27) can be solved iteratively by plugging it into itself. Iterating once, it becomes

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \cdots \int_{t_0}^{\tau_2} d\tau_1 H(\tau_n) H(\tau_{n-1}) \cdots H(\tau_1) \tag{28}$$

Eqn (28) has the time variables as *fully order* $t \leq \tau_n \leq \cdots \leq \tau_1 \leq_0$ and common to use a positive time order exponential denoted as

$$U(t,t_0) = e_+^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau H(\tau)}. \tag{29}$$

Some cases may require taking the Hermitian conjugate

$$U^\dagger(t,t_0) = e_-^{\frac{i}{\hbar}\int_{t_0}^{t} d\tau H(\tau)} \tag{30}$$
$$\langle\psi(t)| = \langle\psi(t)|U^\dagger(t,t_0) \tag{31}$$

Deriving eqn (30) uses the hermiticity of the Hamiltonian $H^\dagger(\tau) = H(\tau)$.

3 Interaction Picture

The time evolution operator is formally expressed and derived as follow

$$|\psi(t)\rangle = U(t,t')U(t',t'')|\psi(t'')\rangle \tag{32}$$
$$U(t,t'') = U(t,t')U(t',t'') \tag{33}$$

The time operator can break it up as many times,

$$U(t,t_0) = U(t,t_n)U(t_n,t_{n-1}) \cdots U(t_1,t_0) \tag{34}$$

This can be written into a large number N of equal time segments δt with $N\Delta t = t - t_0$. If Δt is very small, then

$$U(t_n,t_{n-1}) \approx 1 - \frac{i}{\hbar} H(t_n)\Delta t. \tag{35}$$

Introduced Eqn (35) is the *infinitesimal evolution operator*. Several properties can be shown such as unitary operator and the total time evolution operator is the product of infinitesimal evolution operator

$$U_{\text{tot}}(t,t_0) = \left[1 - \frac{i}{\hbar}H(t_{n-1})\Delta t\right]\left[1 - \frac{i}{\hbar}H(t_{n-2})\Delta t\right]\cdots\left[1 - \frac{i}{\hbar}H(t_0)\Delta t\right] \tag{36}$$

$$\approx 1 - \frac{i}{\hbar}\sum_{j=0}^{n} H(t_j)\Delta t + \cdots \tag{37}$$

$$\approx 1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau H(\tau) \tag{38}$$

The interaction picture allows the Hamiltonian to contain the zeroth order H_0 treated exactly while the remainder $H'(t)$ is expanded perturbatively. Let's solve the H_0 exactly,

$$H(t) = H_0(t) + H'(t) \tag{39}$$

$$\frac{\partial}{\partial t}U_0(t,t_0) = -\frac{i}{\hbar}H_0(t)U_0(t,t_0) \tag{40}$$

$$U_0(t,t_0) = e_+^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau H_0(\tau)} \tag{41}$$

The solution of the $U_0(t,t_0)$ lead to the definition of the interaction picture wavefunction $|\psi_{\text{I}}(t)\rangle$

$$|\psi_S(t)\rangle \equiv U_0(t,t_0)|\psi_I(t)\rangle \tag{42}$$

where $|\psi_S(t)\rangle$ is the Schrödinger picture wavefunction. Substituion of the interaction picture wavefunction into the TDSE yields

$$\frac{\partial|\psi_I(t)\rangle}{\partial t} = -\frac{i}{\hbar}H_I'(t)|\psi_I(t)\rangle \tag{43}$$

$$H_I'(t) \equiv U_0^\dagger(t,t_0)H'(t)U_0(t,t_0) \tag{44}$$

The time propagator operator is introduced within the interaction representation

$$|\psi_I(t)\rangle \equiv U_I(t,t_0)|\psi(t_0)\rangle \tag{45}$$

Upon substituting Eqn (45) into Eqn (43) to get

$$\frac{\partial}{\partial t}U_I(t,t_0) = -\frac{i}{\hbar}H_I'(t)U_I(t,t_0) \tag{46}$$

$$U_I(t,t_0) = e_+^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau H_I'(\tau)} \tag{47}$$

Looking back at the Schrödinger picture, the time propagator operator $U(t,t_0)$ can be derived

$$|\psi_S(t)\rangle = U_0(t,t_0)|\psi_I(t)\rangle \tag{48}$$

$$= U_0(t,t_0)U_I(t,t_0)|\psi_I(t_0)\rangle \tag{49}$$

$$= U_0(t,t_0)U_I(t,t_0)|\psi_S(t_0)\rangle \tag{50}$$

At initial time t_0, the $|\psi_I(t_0)\rangle = |\psi_S(t_0)\rangle$ and hence, the $U(t,t_0)$ becomes

$$U(t,t_0) = U_0(t,t_0)U_I(t,t_0) \tag{51}$$

$$= U_0(t,t_0)e_+^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau H_I'(t)} \tag{52}$$

As long as H_0 and $U_0(t,t_0)$ are expressed exactly, the time operator may be expanded in powers of $H'(\tau)$ alone

$$U(t,t_0) = U_0(t,t_0) + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} d\tau_n \cdots \int_{t_0}^{\tau_2} d\tau_1 U_0(t,\tau_n)H'(\tau_n)U_0(\tau_n\tau_{n-1})\cdots U_0(\tau_2,\tau_1)H'(\tau_2)U_0(\tau_1,t_0). \tag{53}$$

All time ordering is satisfied by Eqn (53). The result may be interpreted as the system propogating freely from time t_0 to τ_1 with $U_0(\tau_1, t_0)$ and then interacts with $H'(\tau_1)$ from time τ_1 to τ_2 with $U_0(\tau_2, \tau_1)$ and etc. In addition, this form allow truncation at low order and propagation at long time. The corresponding wavefunction can be determine up to first order

$$|\psi(t)\rangle = |\psi_0(t)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} d\tau U_0(t,\tau)H'(\tau)|\psi(\tau)\rangle \tag{54}$$

where

$$|\psi_0(t)\rangle \equiv U_0(t,t_0)|\psi_S(t_0)\rangle \tag{55}$$

3.1 Properties of Interaction Picture

The interaction picture has a significant meaning for a given operator A defined as

$$A_I(t) \equiv U_0^\dagger(t,t_0)A_S U(t,t_0) \tag{56}$$

Time evolution in the interaction picture is given by

$$\langle A(t)\rangle = \langle \psi_I(t)|A_I(t)|\psi_I(t)\rangle \tag{57}$$

$$\frac{\partial \psi_I}{\partial t} = -\frac{i}{\hbar}H_I'(t)\psi_I \tag{58}$$

$$\frac{\partial A_I}{\partial t} = \frac{i}{\hbar}[H_0, A_I] \tag{59}$$

$$H_I'(t) = U_0^\dagger(t,t_0)H'(t)U_0(t,t_0) \tag{60}$$

These equations are valid for an arbitrary partitioning of the Hamiltonian. For instance, choosing the $H_0 = 0$ and $H' = H$ yield the *Schrödinger picture* where the time evolution is entirely with the wavefunction and the operators are time independent. Moreover, a choice of $H_0 = H$ and H'=0 yields the *Heisenberg picture* where the wavefunction is time independent and the entire evolution is with the operator. Meanwhile, the interaction picture is the mix beteween the *Schrödinger* and *Heisenberg pictures*.

3.2 Magnus Expansion

The application of the cumulant expansion on the time evolution operator in the interaction picture and expressed the time-ordered exponential of H_I' as an ordinary exponential of a different, time-dependent operator, given by an infinite series.

$$U_I(t,t_0) = e_+^{-i/\hbar\int_0^t d\tau H_I'(\tau)} \equiv e^{\sum_{n=1}^{\infty}(1/n!)(-i/\hbar)^n H_n(t,t_0)} \tag{61}$$

where

$$H_1 = \int_{t_0}^{t} d\tau_1 H_I'(\tau_1) \tag{62}$$

$$H_2 = \int_{t_0}^{t} d\tau_2 \int_{t_0}^{t_2} d\tau_1 [H_I'(\tau_2), H_I'(\tau_1)] \tag{63}$$

$$H_3 = \int_{t_0}^{t} d\tau_3 \int_{t_0}^{t_3} d\tau_2 \int_{t_0}^{t_2} d\tau_1 \{[H_I'(\tau_3), [H_I'(\tau_2), H_I'(\tau_1)]] + [[H_I'(\tau_3), H_I'(\tau_2)], H_I'(\tau_1)]\}. \tag{64}$$

4 Green Function and Casuality

Casuality describes that in the natural science, the effect does not come before the cause. An example is that the effect of a ball moving happens due to a force causing it to move. With the time evolution operator $U(t,t_0)$, it is useful to work in the frequency domain rather than the time domain. This unitary transformation is done by the Green function which separates the forward ($t > t_0$) and reverse ($t < t_0$) propagations.

$$\begin{aligned} G(t-t_0) &\equiv \theta(t-t_0)U(t,t_0) \\ &= \theta(t-t_0)E^{(-i/\hbar)H(t-t_0)} \end{aligned} \tag{65}$$

where $\theta(t-t_0)$ is the Heavyside step function. Contour integration yields

$$\theta(t-t_0)U(t,t_0)7 = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE e^{-(i/\hbar)E(t-t_0)}G(E) \tag{66}$$

$$G(E) = \sum_n \frac{|\phi_n\rangle\langle\phi_n|}{E - E_n + i\epsilon} \tag{67}$$

Once in this form, perturbative expansion can be conveniently carried out using the Green functio which satisfy the Dyson equation. The zero order Green function

$$G_0(E) = \frac{1}{E - H_0 + i\epsilon} \tag{68}$$

where $H = H_0 + V$. Using the identity $A^{-1} = B^{-1}(B - A)A^{-1}$, where A and B are operators, then

$$G(E) = G_0(E) + G_0(E)VG(E) \tag{69}$$

$$G(E) = G_0(E) + G_0(E)VG_0(E) + G_0(E)VG_0(E)VG_0(E) + \cdots \tag{70}$$

Keep in mind, $G_0(E)$ is a diagonal matrix while V is an off-diagonal matrix.