# Propagation with time-dependent Hamiltonian

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**Abstract**

In this note, we introduce one basic concept in nonlinear optical spectroscopy: time-dependent Hamiltonian. Then we give one example of application of the time evolution operator.

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In optical spectroscopy, the choice we face is: (1) working with a time-independent Hamiltonian in a larger phase space that includes the matter and the radiation field(Shaul Mukamel, 1995); (2) using a time-dependent Hamiltonian in a smaller phase space of the matter alone.

For any vector $|\psi\rangle$ in Hilbert space, its dynamical equation is the time-dependent Schrodinger equation:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \mathbf{H}|\psi(t)\rangle. \tag{1}$$

Since

$$|\psi(t)\rangle = \sum_l |f_l\rangle\langle f_l|\psi(t)\rangle, \tag{2}$$

and

$$\mathbf{H}|f_l\rangle = E_l|f_l\rangle, \tag{3}$$

we have

$$i\hbar\frac{\partial}{\partial t}\langle f_l|\psi(t)\rangle = E_l\langle f_l|\psi(t)\rangle,$$

which is

$$i\hbar\frac{\partial}{\partial t}c_l = E_l c_l,$$

or

$$\mathbf{Hc} = E\mathbf{c}.$$

(4)

We obtain the wave function at time $t$:

$$\langle f_l|\psi(t)\rangle = e^{-\frac{iE_l(t-t_0)}{\hbar}}\langle f_l|\psi(t_0)\rangle, \tag{5}$$

where $\langle f_l|\psi(t_0)\rangle$ is the initial expansion coefficients of the wavefunction. We then have

$$|\psi(t)\rangle = \sum_l e^{-\frac{iE_l(t-t_0)}{\hbar}}|f_l\rangle\langle f_l|\psi(t_0)\rangle, \tag{6}$$

Therefore, the evolution operator $U(t,t_0)$ can be defined as:

$$|\psi(t)\rangle \equiv U(t,t_0)|\psi(t_0)\rangle,$$

or

$$U(t,t_0) \equiv \sum_l |f_l\rangle e^{-\frac{iE_l(t-t_0)}{\hbar}}\langle f_l|. \tag{7}$$

It is immediately follows that

$$U(t_0,t_0)| = 1. \tag{8}$$

The eq. 7 gives the evolution operator in a specific representation, i.e., the eigenstates of the Hamiltonian $\mathbf{H}$.

Here is one example of application of the time evolution operator. Calculate the time evolution operator of a coupled 2-level system($|\psi_a\rangle$ and $|\psi_b\rangle$) with energies $\epsilon_a$, $\epsilon_b$, and a coupling $V_{ab}$, represented by the Hamiltonian

$$\begin{bmatrix} \epsilon_a & V_{ab} \\ V_{ba} & \epsilon_b \end{bmatrix}.$$

Solution: Denote

$$V_{ab} = V_{ba}^* = |V_{ab}|e^{-i\chi}(0 < \chi < \pi/2).$$

(9)

Denote $\lambda$ as the eigenvalue of the energy, solve the JiuQi equation

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

(10)

we get the eigenvalue of the energy: $\lambda_\pm = \frac{(\epsilon_a+\epsilon_b)\pm\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}}{2}$. Then the eigenstates can be calculated. For $\lambda = \lambda_-$,

$$(\epsilon_b - \lambda_-)b = -V_{ab}e^{i\chi}a,$$

(11)

i.e.,

$$\frac{b}{a} = \frac{-|V_{ab}|e^{i\chi}}{\epsilon_b - \lambda_-}$$
$$= \frac{-2|V_{ab}|e^{i\chi}}{(\epsilon_b-\epsilon_a)+\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}}$$
$$= \frac{-2|V_{ab}|e^{i\chi}/(\epsilon_a-\epsilon_b)}{-1+\sqrt{1+\frac{4|V_{ab}|^2}{(\epsilon_a-\epsilon_b)^2}}}$$
$$= \frac{-\tan 2\theta}{-1+\sec 2\theta}e^{i\chi}$$
$$= -\frac{\cos\theta}{\sin\theta}e^{i\chi},$$

where we have set

$$\tan 2\theta \equiv \frac{2|V_{ab}|}{\epsilon_a - \epsilon_b}, 0 < \theta < \frac{\pi}{2}. \tag{12}$$

Therefore,

$$|\psi_-\rangle = \begin{bmatrix} -\sin\theta e^{-i\chi/2} \\ \cos\theta e^{i\chi/2} \end{bmatrix}. \tag{13}$$

Similarly, replace $\lambda_-$ by $\lambda_+$, we can obtain

$$|\psi_+\rangle = \begin{bmatrix} \cos\theta e^{-i\chi/2} \\ \sin\theta e^{i\chi/2} \end{bmatrix}.$$

(14)

Thus,from eq. 7, the time evolution operator is

$$U(t,t_0) = |\psi_+\rangle\langle\psi_+|e^{-\frac{i}{\hbar}\lambda_+(t-t_0)} + |\psi_-\rangle\langle\psi_-|e^{-\frac{i}{\hbar}\lambda_-(t-t_0)}. \tag{15}$$

Using eq.( 13) and ( 14), we obtain the exprssion of $U(t,t_0)$:

$$U(t,t_0) =$$

$$\begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta e^{-i\chi} \\ \cos\theta\sin\theta e^{i\chi} & \sin^2\theta \end{bmatrix} \mathrm{e}^{-\frac{i}{\hbar}\lambda_+(t-t_0)} +$$

$+$

$$\begin{bmatrix} \sin^2\theta & -\cos\theta\sin\theta e^{-i\chi} \\ -\cos\theta\sin\theta e^{i\chi} & \cos^2\theta \end{bmatrix} \mathrm{e}^{-\frac{i}{\hbar}\lambda_-(t-t_0)}.$$

(16)

Discussion: suppose the system is initially (at time $t_0 = 0$) in the $|\phi_a\rangle$ state, i.e., $|\psi(0)\rangle = |\phi_a\rangle$. We can calculate the probability of the system to be found in the $|\phi_b\rangle$ state at time $t$

$$P_{ba}(t) = |\langle\phi_b|\psi(t)\rangle|^2 \tag{17}$$
$$= |\langle\phi_b|U(t,t_0)\psi(0)\rangle|^2$$
$$= |\langle\phi_b|U(t,t_0)|\phi_a\rangle|^2$$

(18)

Since

$$\langle\phi_b|U(t,t_0)|\phi_a\rangle =$$

$\begin{bmatrix}0 & 1\end{bmatrix}$

$\begin{bmatrix}U_{aa}(t) & U_{ab}(t)\\ U_{ba}(t) & U_{bb}(t)\end{bmatrix}$

$\begin{bmatrix}1\\0\end{bmatrix}$

= U$_{ba}(t)$

$= \sin\theta\cos\theta e^{i\chi}e^{-\frac{i}{\hbar}\lambda_+(t-t_0)} -$

- $\sin\theta\cos\theta e^{i\chi}e^{-\frac{i}{\hbar}\lambda_-(t-t_0)}$

$= \sin 2\theta e^{i\chi}\frac{}{2(\cos\frac{\lambda_+(t-t_0)}{\hbar} - i\sin\frac{\lambda_+(t-t_0)}{\hbar} -}$

- $\cos\lambda_-(t-t_0)\frac{}{\hbar + i\sin\frac{\lambda_-(t-t_0)}{\hbar})}$

$=\sin 2\theta e^{i\chi}\frac{}{2\times 2i\sin\beta(\cos\alpha - i\sin\alpha)}$

=isin$2\theta e^{i(\chi-\alpha)}\sin\beta$, (13)where we have defined

$$\alpha = \frac{(\epsilon_a+\epsilon_b)(t-t_0)}{2\hbar}, \beta = \frac{\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}(t-t_0)}{2\hbar}.$$

(14)

So

$$|\langle\phi_b|U(t,t_0)|\phi_a\rangle|^2 = \sin^2 2\theta \sin^2\beta$$
$$= \frac{4|V_{ab}|^2}{\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}}\sin^2\frac{\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}(t-t_0)}{2\hbar}. \tag{15}$$

This is known as Rabi formula and

$$\Omega_R \equiv \frac{\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}}{\hbar} \tag{16}$$

is known as Rabi frequency. For example, in the case of alkali atoms, the order of magnitude of the Rabi frequency is MHz. We assume that $(\epsilon_a - \epsilon_b)^2$ and $4|V_{ab}|^2$ have the same order of magnitude, i.e., $\frac{4|V_{ab}|^2}{\sqrt{(\epsilon_a-\epsilon_b)^2+4|V_{ab}|^2}} \sim \sqrt{(\epsilon_a - \epsilon_b)^2 + 4|V_{ab}|^2} \approx 10^6$.

# References


(1995).