13.2: Iterative solution for the interaction-picture state vector

The solution to Equation ??? can be expressed in terms of a unitary propagator $U_I(t;t_0)$, the interaction-picture propagator, which evolves the initial state $|\Phi(t_0)\rangle$ according to

$$|\Phi(t)\rangle = U_I(t;t_0)|\Phi(t_0)\rangle = U_I(t;t_0)|\Psi(t_0)\rangle \tag{13.2.1}$$

Substitution of Equation 13.2.1 into Equation ??? yields an evolution equation for the propagator $U_I(t;t_0)$:

$$H_I(t)U_I(t;t_0) = i\hbar\frac{\partial}{\partial t}U_I(t;t_0) \tag{13.2.2}$$

The initial condition on Equation 13.2.2 is $U_I(t_0;t_0)=I$. In developing a solution to Equation 13.2.2, we assume that $H_I(t)$ is a small perturbation, so that the solution can take the form of a sum of powers of $H_I(t)$.

A solution of this form can be generated by recognizing that Equation 13.2.2 can be solved formally in terms of an integral equation:

$$U_I(t;t_0) = U_I(t_0;t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t')U_I(t';t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t')U_I(t';t_0) \tag{13.2.3}$$

It is straightforward to verify this form solution for $U_I(t;t_0)$. Computing the time derivative of both sides gives

$$i\hbar\frac{\partial}{\partial t}U_I(t;t_0) = -i\hbar\frac{i}{\hbar}\frac{\partial}{\partial t}\int_{t_0}^{t} dt'\ H_I(t')U_I(t';t_0) = H_I(t)U_I(t;t_0) \tag{13.2.4}$$

Thus, Equation 13.2.3 is a valid expression of the solution. The implicit nature of the integral equation means that an iterative procedure based on the assumption that $H_I(t)$ is a small perturbation can be easily developed. We start with a zeroth-order solution by setting $H_I(t)=0$ in Equation 13.2.3, which gives the trivial result

$$U_I^{(0)}(t;t_0) = I \tag{13.2.5}$$

This solution is now fed back into the right side of Equation 13.2.3 to develop a first-order solution:

$$U^{(1)}(t;t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t')U_I^{(0)}(t';t_0) \tag{13.2.6}$$

$$= I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t') \tag{13.2.7}$$

The first order solution is fed back into the right side of Equation 13.2.3 to develop a second-order solution:

$$U^{(2)}(t;t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t')U_I^{(1)}(t';t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t') + \left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\ H_I(t')H_I(t'') \tag{13.2.8}$$

and so forth, such that the k th-order solution is always generated from the $(k-1)$ st-order solution according to the recursion formula:

$$U^{(k)}(t;t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t')U_I^{(k-1)}(t';t_0) \tag{13.2.9}$$

Thus, the third-order solution is given by

$$U^{(2)}(t;t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ H_I(t') + \left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\ H_I(t')H_I(t'') - \left(\frac{i}{\hbar}\right)^3\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\int_{t_0}^{t''} dt'''\ H_I(t')H_I(t'')H_I(t''') \tag{13.2.10}$$

The exact solution is then just a sum of the solutions obtained at each order:

$$U_I(t;t_0) = \sum_{k=0}^{\infty}(-1)^k\left(\frac{i}{\hbar}\right)^k\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\cdots\int_{t_0}^{t^{(k-1)}} dt^{(k)}\ H_I(t')H_I(t'')\cdots H_I(t^{(k)}) \tag{13.2.11}$$

Having seen how to generate a solution for the propagator in the interaction picture to arbitrarily high orders in the perturbation, the time evolution of the state vector $|\Phi(t)\rangle$ in the interaction picture can be determined from

$$|\Phi(t)\rangle = U_I(t;t_0)|\Phi(t_0)\rangle \tag{13.2.12}$$

and from this expression, the time evolution of the original state vector $|\Phi(t)\rangle$ in the Schrödinger picture can be determined

$$|\Phi(t)\rangle = e^{-iH_0(t-t_0)/\hbar}|\Phi(t)\rangle = e^{-iH_0(t-t_0)/\hbar}U_I(t;t_0)|\Phi(t_0)\rangle = e^{-iH_0(t-t_0)/\hbar}U_I(t;t_0)|\Psi(t_0)\rangle \equiv U(t;t_0)|\Psi(t_0)\rangle \tag{13.2.13}$$

where we have used the fact that $|\Phi(t_0)\rangle = |\Psi(t_0)\rangle$ and, in the last line, the full propagator in the Schrödinger picture is identified as

$$U(t;t_0) = e^{-iH_0(t-t_0)/\hbar}U_I(t;t_0) \tag{13.2.14}$$

From Equation 13.2.14, the structure of the full propagator for the time-dependent system reveals itself. Let us use Equation 13.2.14 to generate the first few lowest order terms in the propagator. Substituting Equation 13.2.5 into Equation 13.2.14 yields the lowest order contribution to $U(t;t_0)$:

$$U^{(0)}(t;t_0) = e^{-iH_0(t-t_0)/\hbar} = U_0(t;t_0) \tag{13.2.15}$$

Thus, at zeroth order, Equation 13.2.15 implies that the system is to be propagated using the unperturbed propagator $U_0(t;t_0)$ as if the perturbation did not exist. At first order, we obtain

$$U^{(1)}(t;t_0) = e^{-iH_0(t-t_0)/\hbar} - \frac{i}{\hbar}e^{-iH_0(t-t_0)/\hbar}\int_{t_0}^{t} dt'\ H_I(t') \tag{13.2.16}$$

$$= e^{-iH_0(t-t_0)/\hbar} - \frac{i}{\hbar}e^{-iH_0(t-t_0)/\hbar}\int_{t_0}^{t} dt' e^{-iH_0(t'-t_0)/\hbar}\mathrm{H}_1(t')e^{-iH_0(t'-t_0)/\hbar} \tag{13.2.17}$$

$$= e^{-iH_0(t-t_0)/\hbar} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ e^{-iH_0(t-t')/\hbar}\mathrm{H}_1(t')e^{-iH_0(t'-t_0)/\hbar} \tag{13.2.18}$$

$$= U_0(t;t_0) - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ U_0(t;t')\mathrm{H}_1(t')U_0(t';t_0) \tag{13.2.19}$$

where, in the second line, the definition of $H_I(t)$ in terms of the original perturbation Hamiltonian $H_1(t)$ has been used. What Equation 13.2.19 says is that at first order, the propagator is composed of two terms. The first term is simply the unperturbed propagation from t_0 to t. In the second term, the system undergoes unperturbed propagation from t_0 to t' and at t', the perturbation $H_1(t')$ is allowed to act. From t' to t, the system undergoes unperturbed propagation. Finally, we need to integrate over all possible intermediate times t'.

In a similar manner, it can be shown that up to second order, the full propagator is given by

$$U^{(2)}(t;t_0) = U_0(t;t_0) - \frac{i}{\hbar}\int_{t_0}^{t} d'\ U_0(t;t')\mathrm{H}_1(t')U_0(t';t_0) + \left(\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \\ U_0(t;t')\mathrm{H}_1(t')U_0(t';t'')\mathrm{H}_1(t'')U_0(t'';t_0) \tag{13.2.20}$$

Thus, at second order, the new term involves unperturbed propagation from t_0 to t'', action of $H_1(t'')$ at t'', unperturbed propagation from t'' to t', action of $H_1(t')$ at t' and, finally, unperturbed propagation from t' to t. Again, the intermediate times t' and t'' must be integrated over. The picture on the left side of the equation indicates that the perturbation causes the system to undergo some undetermined dynamical process between t_0 and t. The terms on the right show how that process is broken down in terms of the action of the perturbation H_1 at specific intermediate times. At the k th order, the perturbation Hamiltonian H_1 acts on the system at k specific instances in time. Because of the limits of integration, these time instances are ordered chronologically.

The specific ordering of the instances in time when H_1 acts on the unperturbed system raises an important point. At each order the expansion for $U_I(t;t_0)$, the order in which the operators $H_I(t')$, $H_I(t'')$, etc. are multiplied is important. The reason for this is that the operator $H_I(t)$ does not commute with itself at different instances in time

$$[H_I(t), H_I(t')] \neq 0 \tag{13.2.21}$$

Thus, in order to remove any possible ambiguity when specifying the order in which operators are to be applied in a time series, we introduce the *time-ordering operator*, T. The purpose of T is to take a product string of time-dependent operators $A(t_1)B(t_2)C(t_3)\cdots D(t_n)$ which act at different instances in time $t_1, t_2, \cdots, t_n$ and order the operators in the product such that they act chronologically in time from the earliest time to the latest time. For example, the action of T on two operators $A(t_1)$ and $B(t_2)$ is

$$T\left(A(t_1)B(t_2)\right) = \begin{cases} A(t_1)B(t_2) & t_2 < t_1 \\ B(t_2)A(t_1) & t_1 < t_2 \end{cases} \tag{13.2.22}$$

Let us now apply the time-ordering operator to the second-order term. First write the double integral as a sum of two terms generated simply interchanging the names of the dummy variables t' and t'':

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\ H_I(t')H_I(t'') = \frac{1}{2}\left[\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_I(t')H_I(t'') + \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt'\ H_I(t'')H_I(t')\right] \tag{13.2.23}$$

The same region can be covered by choosing $t' \in [t_0, t]$ and $t'' \in [t_0, t]$. With this choice, Equation 13.2.23 becomes

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') = \frac{1}{2}\left[\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H_I(t') H_I(t'') + \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\, H_I(t'') H_I(t')\right] \tag{13.2.24}$$

In the first term on the right side of Equation 13.2.24, $t'' < t'$ and $H_I(t'')$ acts first, followed by $H_I(t')$. In the second term, $t' < t''$ and $H_I(t')$ acts first followed by $H_I(t'')$. The two terms can, thus, be combined with both t' and t'' lying in the interval $[t_0, t]$ if the time-ordering operator is applied:

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, H_I(t') H_I(t'') = \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, T\left(H_I(t') H_I(t'')\right) \tag{13.2.25}$$

The same analysis can be applied to each order in Equation 13.2.11, recognizing that the number of possible time orderings of a product of k operators is $k!$. Thus, Equation 13.2.11can be rewritten in terms of the time-ordering operator as

$$U_I(t;t_0) = \sum_{k=0}^{\infty} (-1)^k \left(\frac{i}{\hbar}\right)^k \frac{1}{k!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_k T\left(H_I(t_1) H_I(t_2) \cdots H_I(t_k)\right) \tag{13.2.26}$$

The sum in Equation 13.2.26resembles the power-series expansion of an exponential, and, indeed, we can write the sum symbolically as

$$U_I(t;t_0) = T\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H_I(t')\right)\right] \tag{13.2.27}$$

which is known as a *time-ordered exponential*. Equation 13.2.27 is really a symbolic representation of Equation 13.2.26, in which it is understood that the time-ordering operator acts to order the operators in each term of the expansion of the exponential.

Given the formalism of time-dependent perturbation theory, we now seek to answer the following question: If the system is initially in an eigenstate of H_0 with energy E_i, what is the probability as a function of time t that the system will undergo a transition to a new eigenstate of H_0 with energy E_f? From the statement of the question, it is clear that the initial state vector $|\Psi(t_0)\rangle$ is simply the eigenstate of H_0 with energy E_i

$$|\Psi(t_0)\rangle = |E_i\rangle \tag{13.2.28}$$

The amplitude as a function of time that the system will undergo a transition to the eigenstate $|E_f\rangle$ is obtained by propagating this initial state out to time t with the propagator $U(t;t_0)$ and then taking the overlap of the resultant state with the eigenstate $|E_f\rangle$:

$$A_{fi}(t) = \langle E_f | U(t;t_0) | E_i\rangle \tag{13.2.29}$$

and the probability is just the square magnitude of this complex amplitude:

$$P_{fi}(t) = |\langle E_f | U(t;t_0) | E_i\rangle|^2 \tag{13.2.30}$$

Consider, first, the amplitude at zeroth order in perturbation theory. At this order, $U(t;t_0) = U_0(t;t_0)$, and the amplitude is simply

$$A_{fi}^{(0)}(t) = \langle E_f | e^{-iH_0(t-t_0)/\hbar} | E_i\rangle \tag{13.2.31}$$

$$= e^{-iE_i(t-t_0)/\hbar}\langle E_f | E_i\rangle \tag{13.2.32}$$

which clearly vanishes if $E_i \neq E_f$. Thus, at zeroth order, the only possibility is the trivial one in which no transition occurs.

The lowest nontrivial order is first order, where the transition amplitude is given by

$$A_{fi}^{(1)}(t) = \langle E_f | U^{(1)}(t;t_0) | E_i\rangle = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, \langle E_f | U_0(t;t') \mathrm{H}_1(t') U_0(t';t_0) | E_i\rangle \tag{13.2.33}$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt\, \langle E_f | e^{-iH_0(t-t')/\hbar} \mathrm{H}_1(t') e^{-iH_0(t'-t_0)/\hbar} | E_i\rangle \tag{13.2.34}$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, e^{-iE_f(t-t')/\hbar} e^{-iE_i(t'-t_0)/\hbar}\langle E_f | \mathrm{H}_1(t') | E_i\rangle \tag{13.2.35}$$

$$= -\frac{i}{\hbar} e^{-iE_f t/\hbar} e^{iE_i t_0/\hbar}\int_{t_0}^{t} dt'\, e^{i(E_f - E_i)t'/\hbar}\langle E_f | \mathrm{H}_1(t') | E_i\rangle \tag{13.2.36}$$

Define a transition frequency ω_{fi} by

$$\omega_{fi} = \frac{E_f - E_i}{\hbar} \tag{13.2.37}$$

Then, taking the absolute square of the last line of Equation 13.2.36, we obtain the probability at first-order

$$P_{fi}^{(1)}(t) = \frac{1}{\hbar^2}\left|\int_{t_0}^{t} dt' e^{i\omega_{fi}t'}\langle E_f|\mathrm{H}_1(t')|E_i\rangle\right|^2 \tag{13.2.38}$$

At first order, the probability depends on the matrix element of the perturbation between the initial and final eigenstates. Thus far, the formalism we have derived is valid for any perturbation Hamiltonian $H_1(t)$. If we consider the use of an external perturbation to probe the eigenvalue spectrum of H_0, then the specific type of probe determines the form of $H_1(t)$, as we saw in the first section and will explore in the next subsection.
