TIME-DEPENDENT PERTURBATION THEORY: ITERATIVE SOLUTION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 9.4.

We've seen that we can solve the Schrödinger equation with a time-dependent potential in a two-state system if we split the hamiltonian into a time-independent part H^0 and a time-dependent part H', so that the complete hamiltonian is

$$H = H^0 + H' \tag{1}$$

The solution is

$$\Psi(x,t) = c_a(t)\,\psi_a(x)\,e^{-iE_at/\hbar} + c_b(t)\,\psi_b(x)\,e^{-iE_bt/\hbar} \tag{2}$$

where ψ_a and ψ_b are the two eigenstates of H^0 and the coefficients are solutions of the coupled ODEs

$$\dot{c}_a = -\frac{i}{\hbar}\left[c_a H'_{aa} + c_b H'_{ab} e^{-i(E_b-E_a)t/\hbar}\right] \tag{3}$$

$$\dot{c}_b = -\frac{i}{\hbar}\left[c_b H'_{bb} + c_a H'_{ba} e^{i(E_b-E_a)t/\hbar}\right] \tag{4}$$

where

$$H'_{ij} \equiv \langle\psi_i|H'\left|\psi_j\right\rangle \tag{5}$$

We haven't made any approximations in these equations, but in general we also can't solve them exactly for most perturbations H'. If H' is small compared to H^0, however, we can use various perturbation techniques to get an approximate solution. Conceptually, one of the easiest techniques is that of *iterative solution*.

We begin with a zeroth-order solution in which we specify the initial conditions $c_a(0)$ and $c_b(0)$ and ignore H' completely. Since H' is the only time-dependent part of the hamiltonian, c_a and c_b remain constant for all time. If the system starts out in state ψ_a, for example, then the zeroth order solution is

$$c_a^{(0)}(t) = 1 \tag{6}$$

$$c_b^{(0)}(t) = 0 \tag{7}$$

We can then plug these into the RHS of 3 and 4 (with H' switched on again) to get the first-order solutions:

$$\dot{c}_a^{(1)} = -\frac{i}{\hbar}\left[c_a^{(0)}H'_{aa} + c_b^{(0)}H'_{ab}e^{-i(E_b-E_a)t/\hbar}\right] \tag{8}$$

$$= -\frac{i}{\hbar}H'_{aa} \tag{9}$$

$$c_a^{(1)}(t) = 1 - \frac{i}{\hbar}\int_0^t H'_{aa}\left(t'\right)dt' \tag{10}$$

$$\dot{c}_b^{(1)} = -\frac{i}{\hbar}\left[c_b^{(0)}H'_{bb} + c_a^{(0)}H'_{ba}e^{i(E_b-E_a)t/\hbar}\right] \tag{11}$$

$$= -\frac{i}{\hbar}H'_{ba}e^{i(E_b-E_a)t/\hbar} \tag{12}$$

$$c_b^{(1)}(t) = -\frac{i}{\hbar}\int_0^t H'_{ba}\left(t'\right)e^{i(E_b-E_a)t'/\hbar}dt' \tag{13}$$

where we've used the initial conditions to determine the constants of integration in both cases.

We can then take these values and insert them back on the RHS to get the second order solutions and so on. These solutions aren't exact, since (except for the zeroth order values) we don't have $\left|c_a^{(i)}\right|^2 + \left|c_b^{(i)}\right|^2 = 1$, but we do satisfy this condition to the order of the approximation in each case. For first order

$$\left|c_a^{(1)}\right|^2 + \left|c_b^{(1)}\right|^2 = 1 - \frac{i}{\hbar}\int_0^t H'_{aa}\left(t'\right)dt' + \frac{i}{\hbar}\int_0^t H'_{aa}\left(t'\right)dt' + \mathcal{O}\left(\left(H'\right)^2\right) \tag{14}$$

$$= 1 + \mathcal{O}\left(\left(H'\right)^2\right) \tag{15}$$

where in the first line on the RHS, the third term is the complex conjugate of the second, remembering that $\left(H'_{aa}\right)^* = \left(H'_{aa}\right)$ for hermitian operators.

An alternative method of solving for the coefficients is using the auxiliary variables:

$$d_a \equiv e^{i\int_0^t H'_{aa}(t')dt'/\hbar} c_a \tag{16}$$
$$d_b \equiv e^{i\int_0^t H'_{bb}(t')dt'/\hbar} c_b \tag{17}$$

Taking time derivatives, we get

$$\dot{d}_a = \left(\frac{i}{\hbar}H'_{aa}(t)\,c_a + \dot{c}_a\right) e^{i\int_0^t H'_{aa}(t')dt'/\hbar} \tag{18}$$
$$= -\frac{i}{\hbar}c_b H'_{ab} e^{-i\omega_0 t} e^{i\int_0^t H'_{aa}(t')dt'/\hbar} \tag{19}$$
$$= -\frac{i}{\hbar}e^{-i\omega_0 t} H'_{ab} c_b e^{i\int_0^t \left[H'_{aa}(t') - H'_{bb}(t') + H'_{bb}(t')\right]dt'/\hbar} \tag{20}$$
$$= -\frac{i}{\hbar}e^{-i\omega_0 t} H'_{ab} e^{i\phi} d_b \tag{21}$$

where

$$\phi \equiv \frac{1}{\hbar}\int_0^t \left[H'_{aa}(t') - H'_{bb}(t')\right] dt' \tag{22}$$
$$\omega_0 \equiv \frac{E_b - E_a}{\hbar} \tag{23}$$

and we've used 3 in 19. By a similar calculation using 4 we get

$$\dot{d}_b = -\frac{i}{\hbar}e^{i\omega_0 t} H'_{ba} e^{-i\phi} d_a \tag{24}$$

The equations for d_a and d_b have the same form as those we got for a system in which the diagonal elements H'_{aa} and H'_{bb} are zero, with the complex exponential being $e^{i(\omega_0 - \phi)t}$ instead of just $e^{i\omega_0 t}$. From the definitions 16 and 17 we get the initial conditions

$$d_a(0) = c_a(0) = 1 \tag{25}$$
$$d_b(0) = c_b(0) = 0 \tag{26}$$

We could solve these two ODEs for d_a and d_b as we did earlier and get the exact solution, but if we're interested only in a first-order solution, we can use the iterative technique above. The zeroth order solution is

$$d_a^{(0)}(t) = 1 \tag{27}$$
$$d_b^{(0)}(t) = 0 \tag{28}$$

Using 10 and 13 for $d_{a,b}$ with $H'_{aa}=H'_{bb}=0$ we get

$$d_a^{(1)}(t) = 1 \tag{29}$$

$$d_b^{(1)}(t) = -\frac{i}{\hbar}\int_0^t H'_{ba}\left(t'\right)e^{i(\omega_0-\phi)t'}dt' \tag{30}$$

Now, using 16 and 17 (where H'_{aa} and H'_{bb} are *not* zero, since we're back to the original system), we get

$$c_a^{(1)}(t) = e^{-i\int_0^t H'_{aa}(t')dt'/\hbar} \tag{31}$$

$$c_b^{(1)}(t) = -e^{-i\int_0^t H'_{bb}(t')dt'/\hbar}\frac{i}{\hbar}\int_0^t H'_{ba}\left(t'\right)e^{i(\omega_0-\phi)t'}dt' \tag{32}$$

To first order, $e^x = 1+x+\mathcal{O}\left(x^2\right)$ so to first order, these equations give

$$c_a^{(1)}(t) = 1-\frac{i}{\hbar}\int_0^t H'_{aa}\left(t'\right)dt' + \mathcal{O}\left(\left(H'\right)^2\right) \tag{33}$$

$$c_b^{(1)}(t) = -\frac{i}{\hbar}\int_0^t H'_{ba}\left(t'\right)e^{i(\omega_0-\phi)t'}dt' + \mathcal{O}\left(\left(H'\right)^2\right) \tag{34}$$

Thus to first order, these results agree with 10 and 13.

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