

Laplace transform example 2

Let $\hat{H}(\mathbf{r}, t)$ be the Hamiltonian

$$\hat{H}(\mathbf{r}, t) = \hat{H}_0(\mathbf{r}) + \hat{H}_1(\mathbf{r}, t)$$

where

$$\hat{H}_0\psi_a = E_a\psi_a, \quad \hat{H}_0\psi_b = E_b\psi_b, \quad \hat{H}_0\Psi = (E_a + E_b)\Psi$$

Let $\Psi(\mathbf{r}, t)$ be the following wave function for a two state system.

$$\Psi(\mathbf{r}, t) = \psi_a(\mathbf{r})c_a(t) \exp(-\frac{i}{\hbar}E_a t) + \psi_b(\mathbf{r})c_b(t) \exp(-\frac{i}{\hbar}E_b t)$$

From the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$

we obtain the differential equations

$$\frac{d}{dt}c_a(t) = H_{aa}c_a(t) + H_{ab}c_b(t) \exp(-i\omega_0 t) \quad (1)$$

$$\frac{d}{dt}c_b(t) = H_{bb}c_b(t) + H_{ba}c_a(t) \exp(i\omega_0 t) \quad (2)$$

where

$$H_{ij} = -\frac{i}{\hbar} \langle \psi_i | \hat{H}_1 | \psi_j \rangle, \quad \omega_0 = \frac{E_b - E_a}{\hbar}$$

Solve equations (1) and (2) with initial conditions $c_a(0) = 1$ and $c_b(0) = 0$.

Start with the following Laplace transforms for (1) and (2).

$$sC_a(s) - c_a(0) = H_{aa}C_a(s) + H_{ab}C_b(s + i\omega_0) \quad (3)$$

$$sC_b(s) - c_b(0) = H_{bb}C_b(s) + H_{ba}C_a(s - i\omega_0) \quad (4)$$

Use equation (3) to solve for $C_a(s)$ with $c_a(0) = 1$.

$$C_a(s) = \frac{H_{ab}C_b(s + i\omega_0)}{s - H_{aa}} + \frac{1}{s - H_{aa}}$$

Solve for $C_a(s - i\omega_0)$.

$$C_a(s - i\omega) = \frac{H_{ab}C_b(s)}{s - i\omega_0 - H_{aa}} + \frac{1}{s - i\omega_0 - H_{aa}} \quad (5)$$

Substitute (5) into (4) to obtain

$$sC_b(s) - c_b(0) = H_{bb}C_b(s) + H_{ba} \left(\frac{H_{ab}C_b(s)}{s - i\omega_0 - H_{aa}} + \frac{1}{s - i\omega_0 - H_{aa}} \right)$$

It follows that for $c_b(0) = 0$

$$C_b(s) \left[s - H_{bb} - \frac{H_{ab}H_{ba}}{s - i\omega_0 - H_{aa}} \right] = \frac{H_{ba}}{s - i\omega_0 - H_{aa}}$$

Hence

$$C_b(s) = \frac{H_{ba}}{s^2 - (H_{aa} + H_{bb} + i\omega_0)s + H_{aa}H_{bb} - H_{ab}H_{ba} + iH_{bb}\omega_0}$$

Inverse Laplace transform:

$$\frac{1}{s^2 + as + b} \Rightarrow \frac{2}{k} \sin\left(\frac{kt}{2}\right) \exp\left(-\frac{at}{2}\right), \quad k = \sqrt{4b - a^2}$$

Hence for

$$a = -(H_{aa} + H_{bb} + i\omega_0), \quad b = H_{aa}H_{bb} - H_{ab}H_{ba} + iH_{bb}\omega_0$$

we have

$$c_b(t) = \frac{2H_{ba}}{k} \sin\left(\frac{kt}{2}\right) \exp\left(-\frac{at}{2}\right)$$

Use equation (2) to solve for $c_a(t)$.

$$c_a(t) = \left[\cos\left(\frac{kt}{2}\right) - \frac{a + 2H_{bb}}{k} \sin\left(\frac{kt}{2}\right) \right] \exp(-i\omega_0 t) \exp\left(-\frac{at}{2}\right)$$

For the typical case of $H_{aa} = H_{bb} = 0$ we have

$$c_a(t) = \left[\cos\left(\frac{kt}{2}\right) + \frac{i\omega_0}{k} \sin\left(\frac{kt}{2}\right) \right] \exp\left(-\frac{i\omega_0 t}{2}\right) \quad (6)$$

$$c_b(t) = \frac{2H_{ba}}{k} \sin\left(\frac{kt}{2}\right) \exp\left(\frac{i\omega_0 t}{2}\right) \quad (7)$$