

Two state system

Consider the TD-SE for two level system:

$$\begin{aligned} i\hbar\dot{c}_0 &= E_0c_0 - i\hbar d_{01}c_1 \\ i\hbar\dot{c}_1 &= -i\hbar d_{10}c_0 + E_1c_1 \end{aligned} \quad (1)$$

Introduce new variables:

$$a_i = -i\frac{E_i}{\hbar}, \quad (2)$$

$$b = -d_{01}. \quad (3)$$

The Eqs. (1) then turn to:

$$\begin{aligned} \dot{c}_0 &= a_0c_0 + bc_1 \\ \dot{c}_1 &= -bc_0 + a_1c_1 \end{aligned} \quad (4)$$

Assuming that a_i and b are constant (do not depend on time), by taking second time-derivative we obtain:

$$\begin{aligned} \ddot{c}_0 &= a_0\dot{c}_0 + b\dot{c}_1 = a_0(a_0c_0 + bc_1) + b(-bc_0 + a_1c_1) = \\ &= (a_0^2 - b^2)c_0 + (a_0 + a_1)bc_1 = (a_0^2 - b^2)c_0 + (a_0 + a_1)(\dot{c}_0 - a_0c_0), \end{aligned} \quad (5)$$

or

$$\ddot{c}_0 - (a_0 + a_1)\dot{c}_0 + [a_0(a_0 + a_1) - (a_0^2 - b^2)]c_0 = 0, \quad (6)$$

or, finally

$$\ddot{c}_0 - (a_0 + a_1)\dot{c}_0 + (a_0a_1 + b^2)c_0 = 0. \quad (7)$$

To solve the second-order ODE Eq. (7) we assume the following ansatz:

$$c_0 \sim \exp(\alpha t). \quad (8)$$

Substitution of Eq. (8) into Eq. (7) gives the quadratic equation:

$$\alpha^2 - \alpha(a_0 + a_1) + (a_0a_1 + b^2) = 0. \quad (9)$$

with the roots

$$\alpha_{1,2} = \frac{(a_0 + a_1) \pm \sqrt{(a_0 + a_1)^2 - 4(a_0a_1 + b^2)}}{2} = \frac{(a_0 + a_1) \pm \sqrt{(a_0 - a_1)^2 - 4b^2}}{2}. \quad (10)$$

Each of the roots gives the specific solution of the ODE Eq. (7). The general solution is obtained by summing specific solutions with some coefficients:

$$c_0(t) = A \exp(\alpha_1 t) + B \exp(\alpha_2 t) = \exp\left(\frac{(a_0 + a_1)}{2} t\right) [A \exp(i\Omega t) + B \exp(-i\Omega t)], \quad (11)$$

where

$$\Omega = \frac{\sqrt{4b^2 - (a_0 - a_1)^2}}{2} = \sqrt{b^2 - \left(\frac{a_0 - a_1}{2}\right)^2} = \sqrt{b^2 + \left(\frac{E_0 - E_1}{2\hbar}\right)^2}. \quad (12)$$

The coefficients are determined by the initial conditions. For example

If $c_0(t) = 0$, then $B = -A$ and solution Eq. (11) takes the form:

$$c_0(t) = A \exp\left(\frac{(a_0 + a_1)}{2}t\right) [\exp(i\Omega t) - \exp(-i\Omega t)] = 2iA \exp\left(\frac{(a_0 + a_1)}{2}t\right) \sin(\Omega t). \quad (13)$$

The population of the considered state (0) is then given by:

$$|c_0(t)|^2 = 4A^2 \sin^2(\Omega t). \quad (14)$$

The exponent disappears because a_i are the pure imaginary quantities.

The transition rate can be obtained as:

$$r_{1 \rightarrow 0} = \frac{d}{dt} |c_0(t)|^2 = 8A^2 \Omega \sin(\Omega t) \cos(\Omega t) = 4\Omega A^2 \sin(2\Omega t). \quad (15)$$

This shows that the population oscillates with some frequency, depending on the energy difference of two levels $E_0 - E_1$ and the coupling between them $b = -d_{01}$. For the degenerate case $E_0 - E_1 = 0$ the rate is determined only by the coupling d_{01} . Alternatively, if the states are not coupled $d_{01} = 0$ the rate of population transfer is determined only by the energy difference $E_0 - E_1$ - this is a qualitatively incorrect result, because the derivation scheme does not work under such conditions – see the paradox and its solution.

Some asymptotic analysis: using $\sin x \approx x$ we can find that at short times $\Omega t \rightarrow 0$:

$$r_{1 \rightarrow 0} = 4\Omega A^2 \sin(2\Omega t) \approx 8tA^2 \Omega^2 = 8tA^2 \left(b^2 + \left(\frac{E_0 - E_1}{2\hbar} \right)^2 \right). \quad (16)$$

A paradox:

If we assume the states are not coupled ($d_{01} = 0$) in the very beginning of the derivation, the equation (1) will read:

$$\begin{aligned} \dot{c}_0 &= a_0 c_0 \\ \dot{c}_1 &= a_1 c_1 \end{aligned} \quad (17)$$

leading straight to the solution:

$$c_0(t) = c_0(0) \exp(a_0 t) = c_0(0) \exp\left(-i \frac{E_0}{\hbar} t\right), \quad (18)$$

so the population is conserved over time:

$$|c_0(t)|^2 = |c_0(0)|^2. \quad (19)$$

Solving the paradox:

If $d_{01} = 0 \Rightarrow b = 0$, then the substitution in Eq. (5) is invalid, that is the $b\dot{c}_1$ and bc_1 should be set to zero, leading to

$$\ddot{c}_0 = a_0 \dot{c}_0 + b \dot{c}_1 = a_0 \dot{c}_0 = a_0^2 c_0. \quad (20)$$

The equation Eq. (20) has the same solution as Eqs. (17), what solves the paradox.