Time-dependent pearturbation

What we have considered so far

perturbation $\hat{H}'$ is turned on slowly, system can stabilize

no perturbation

$\hat{H}_0$

$\hat{H}_0 + \hat{H}'$

Energy levels can shift, states can mix a little

Suppose now we are introducing a <u>time-dependent</u> perturbation $\hat{H}'(t)$ (i.e we now want to trace the dynamics of the system evolution)

Two-level system: simplest QM model

E_b, ψ_b

E_a, ψ_a

$\hat{H}_0$

$\hat{H}_0 \psi_{a,b} = E_{ab} \psi_{ab}$

Eigenstates are the stationary states $\psi_{ab}(t) = \psi_{a,b} \cdot e^{-iE_{a,b}t/\hbar}$

However, the time-independent Schrodinger equation is a special case of a general Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}_0 \psi$$

We can describe any solution of this equation as a linear combination of ψ_a & ψ_b

$$\psi = c_a \psi_a + c_b \psi_b$$

and $\psi(t) = c_a \psi_a(t) + c_b \psi_b(t) =$

$$= c_a \psi_a e^{-iE_a t/\hbar} + c_b \psi_b e^{-iE_b t/\hbar}$$

For such wave function c_a and c_b are constants, describing the probability of finding our system in each state

$$p_a(t) = p_a = |c_a|^2 , \quad p_b(t) = p_b = |c_b|^2$$

So far we always considered a closed systems, in which no external forces acted, so there was nothing to change the state and shuffle a particle b/w the states.

However, that's what the time-dependent perturbation will do!

If the perturbation depends on time, we must work with the time-dependent Schrodinger equation

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \hat{H}\psi(t) = (\hat{H}_0 + \hat{H}'(t))\,\psi(t)$$

$$\psi(t) = \underline{c_a(t)}\,\psi_a e^{-iE_at/\hbar} + \underline{c_b(t)}\,\psi_b e^{-iE_bt/\hbar}$$

Our goal is to find $c_{a,b}(t)$; we usually assume that at $t=0$ $c_a = 1$, $c_b = 0$ (initial conditions)*

* Note: depending on the time-dependence of $\hat{H}'(t)$, sometimes it make sense to choose $t = -\infty$ as the initial condition, or any other time before the perturbation started, so that the state of the system was well-defined

Let's do some math:

$$\frac{\partial\psi(t)}{\partial t} = \dot{c}_a \psi_a e^{-iE_a t/\hbar} - \frac{iE_a}{\hbar} c_a \psi_a e^{-iE_a t/\hbar} + $$
$$+ \dot{c}_b \psi_b e^{-iE_b t/\hbar} - \frac{iE_b}{\hbar} c_b \psi_b e^{-iE_b t/\hbar}$$

$$\hat{H}_0 \psi = c_a E_a \psi_a e^{-iE_a t/\hbar} + c_b E_b \psi_b e^{-iE_b t/\hbar}$$
$$\hat{H}' \psi = c_a (\hat{H}'\psi_a) e^{-iE_a t/\hbar} + c_b (\hat{H}'\psi_b) e^{-iE_b t/\hbar}$$

$$i\hbar \frac{\partial\psi(t)}{\partial t} = i\hbar \dot{c}_a \psi_a e^{-iE_a t/\hbar} + i\hbar \dot{c}_b \psi_b e^{-iE_b t/\hbar} + \cancel{E_a c_a \psi_a e^{-iE_a t/\hbar}} + \cancel{E_b c_b \psi_b e^{-iE_b t/\hbar}}$$

$$= \cancel{c_a E_a \psi_a e^{-iE_a t/\hbar}} + \cancel{c_b E_b \psi_b e^{-iE_b t/\hbar}} + c_a (\hat{H}'\psi_a) e^{-iE_a t/\hbar} + c_b (\hat{H}'\psi_b) e^{-iE_b t/\hbar}$$

Taking an inner product with ψ_a

$$i\hbar \dot{c}_a \overbrace{\langle\psi_a|\psi_a\rangle}^{=1} e^{-iE_a t/\hbar} + i\hbar \dot{c}_b \overbrace{\langle\psi_a|\psi_b\rangle}^{=0} e^{-iE_a t/\hbar} =$$
$$= c_a \langle\psi_a|\hat{H}'(t)|\psi_a\rangle e^{-iE_a t/\hbar} + c_b \langle\psi_a|\hat{H}'(t)|\psi_b\rangle e^{-iE_b t/\hbar}$$

$$i\hbar \dot{c}_a e^{-iE_a t/\hbar} = c_a \langle\psi_a|\hat{H}'(t)|\psi_a\rangle e^{-iE_a t/\hbar} + c_b \langle\psi_a|\hat{H}'(t)|\psi_b\rangle e^{-iE_b t/\hbar}$$
$$\dot{c}_a \equiv \frac{dc_a}{dt} = \frac{1}{i\hbar} c_a \underbrace{\langle\psi_a|\hat{H}'(t)|\psi_a\rangle}_{H'_{aa} \text{ or } V_{aa}(t)} + \frac{1}{i\hbar} c_b \underbrace{\langle\psi_a|\hat{H}'(t)|\psi_b\rangle}_{H'_{ab} \text{ or } V_{ab}(t)} e^{-i(E_b-E_a)t/\hbar}$$

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

$$\dot{c}_b = \frac{1}{i\hbar} H'_{bb}(t) c_b + \frac{1}{i\hbar} H'_{ba} c_b e^{-i(E_a-E_b)t/\hbar}$$

For many cases the diagonal elements vanish: $H'_{aa} = H'_{bb} = 0$

$$\dot{c}_a = \frac{1}{i\hbar} H'_{ab} c_b e^{-i\omega_0 t} \qquad \omega_0 = \frac{E_b - E_a}{\hbar}$$
$$\dot{c}_b = \frac{1}{i\hbar} H'_{ba} c_a e^{i\omega_0 t}$$

These are exact equations, so far we made no assumptions about the perturbations being small.

Just like before, we will be looking for a solution as a series of consecutively reducing corrections $c_{a,b}(t) = c_{a,b}^{(0)} + c_{a,b}^{(1)} + c_{a,b}^{(2)} + \ldots$

where $c_{a,b}^{(0)} = c_{a,b}(t=0)$ – initial state of the system (no effect of the perturbation)

In our case $\begin{cases} c_a^{(0)} = c_a(t=0) = 1 \\ c_b^{(0)} = c_b(t=0) = 0 \end{cases}$

First-order correction is linear in $\hat{H}'$, the second-order correction expression include $\hat{H}'$ twice, ... etc.

Since
$$\dot{c}_a = -\frac{i}{\hbar} \hat{H}'_{ab} c_b e^{-i\omega_0 t}$$
$$\dot{c}_b = -i/\hbar \, \hat{H}'_{ba} c_a e^{i\omega_0 t}$$

in order to keep the terms of the same order n on both sides of the eqn, we must use the $(n-1)$ order expressions for $c_{a,b}$ coefficients on the right side, since they are multiplied by an extra H_{ab} or H_{ba}

$$\begin{cases} \dot{c}_a^{(n)} = -\frac{i}{\hbar} \hat{H}'_{ab}(t) \, c_b^{(n-1)} e^{-i\omega_0 t} \\ \dot{c}_b^{(n)} = -\frac{i}{\hbar} \hat{H}'_{ba}(t) \, c_a^{(n-1)} e^{i\omega_0 t} \end{cases}$$

First-order correction:

$$\dot{c}_a^{(1)} = -\frac{i}{\hbar} H'_{ab}(t) \, c_b^{(0)} e^{-i\omega_0 t} = 0 \quad (c_b^{(0)} = 0)$$

$\dot{c}_a^{(1)} = 0 \Rightarrow c_a(t) = \text{const} = 0$ no first-order time-dependent correction

$$\dot{c}_b^{(1)} = -\frac{i}{\hbar} H'_{ba}(t) \, c_a^{(0)} e^{i\omega_0 t} = -\frac{i}{\hbar} H_{ba}(t) e^{i\omega_0 t}$$

$$c_b^{(1)}(t) = -\frac{i}{\hbar} \int_0^t H_{ba}(t') e^{i\omega_0 t'} dt'$$

Second - order correction

$$c_a^{(2)}(t) = -\frac{i}{\hbar} H'_{ab}(t) \underbrace{c_b^{(1)}(t)} e^{-i\omega_0 t} =$$

$$= -\frac{i}{\hbar} H'_{ab}(t) e^{-i\omega_0 t} \left(-\frac{i}{\hbar}\right) \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'$$

Thus

$$c_a^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \cdot \int_0^t H'_{ab}(t') e^{-i\omega_0 t'} dt' \int_0^{t'} H'_{ba}(t'') e^{i\omega_0 t''} dt''$$

$$c_b^{(2)}(t) = 0 \qquad \text{(no even- order correction)}$$

So, up to the second order

$$c^{(a)}(t) = 1 - \frac{1}{\hbar^2} \int_0^t H'_{ab}(t') e^{-i\omega_0 t'} dt' \int_0^{t'} H'_{ba}(t'') e^{i\omega_0 t''} dt''$$

$$c^{(b)}(t) = -\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'$$