4. Time Dependent Problems

SS 2024

AQM

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Until now (and probably for large part of your Quantum Mechanics course) we have always considered time INDEPENDENT problems

Much of the interesting physics we can understand through QM has to do with TIME DEPENDENT

INTERACTIONS & PHENOMENA : RADIATION

SCATTERING / COLLISIONS

etc

Consider a system whose Hamiltonian reads

$$H = \underbrace{H_0}_{\text{time independent}} + \underbrace{V(t)}_{\text{time dependent}}$$

Where for now $V(t)$ is **NOT SMALL**

Nevertheless, assume we know full solution to time independent problem, i.e.

$$\underline{\mathcal{H}_0 |n\rangle = E_n |n\rangle}$$

We would like to establish a formalism to study how a general state $|\psi\rangle$ evolves as time passes due to $V(t)$.

@ $t = t_0$ (some arbitrary initial time)

$$|\psi\rangle = \sum_n c_n(t_0) |n\rangle$$

Complete set !

we PARAMETRIZE then its time-evolution as:

$$|\psi; t\rangle = \sum_n c_n(t) e^{-iE_n t/\hbar} |n\rangle$$

we explicitly factored out "trivial" time dependence which exists also if $V(t) = 0$

the $c_n(t)$ so defined is such that if $V(t) = 0$

$$c_n(t) \equiv c_n(t_0)$$

To derive differential equation satisfied by $c_n(t)$ is convenient to introduce INTERACTION PICTURE

" In between " Schrödinger & Heisenberg reprs.

Schrödinger Picture — Heisenberg Picture

$$|\psi; t\rangle_S \longrightarrow |\psi\rangle_H = e^{iHt/\hbar} |\psi; t\rangle_S$$

$$O_S \longrightarrow O(t)_H = e^{iHt/\hbar} O_S \, e^{-iHt/\hbar}$$

Interaction Picture factors out only H_0

$$\left.\begin{aligned} |\psi; t\rangle_I &= e^{iH_0 t/\hbar} |\psi; t\rangle_S \\ O_I &= e^{iH_0 t/\hbar} O_S \, e^{-iH_0 t/\hbar} \end{aligned}\right\}$$

Clearly at $t=0$ $|\psi\rangle_I = |\psi\rangle_S$

NOTICE :

CONVENTIONS for phases for generic "t_0" :

Imagine system is in Energy Eigenstate $|n\rangle$

$$H_0|n\rangle = E_n|n\rangle$$

$\Rightarrow$ In Schrödinger picture, state fixed up to a "phase" "$e^{-iE_n t/\hbar}$"

it is then convenient to pick

$$|i, t_0\rangle_I \equiv |i\rangle$$

$$\Rightarrow |i, t_0\rangle_S = \underset{\substack{\Uparrow \\ \text{phase difference}}}{e^{-iE_i t_0/\hbar}} |i\rangle$$

how does $|\psi;t\rangle_I$ evolve ?

$$i\hbar \frac{\partial}{\partial t}|\psi;t\rangle_I = i\hbar\frac{\partial}{\partial t}\left[e^{iH_0t/\hbar}|\psi,t\rangle_S\right]$$

$$= -\cancel{H_0}\, e^{iH_0t/\hbar}|\psi;t\rangle_S + e^{iH_0t/\hbar}\left[\cancel{H_0}+V\right]|\psi;t\rangle_S$$

$$= \underbrace{e^{iH_0t/\hbar}\, V\, e^{-iH_0t/\hbar}}_{V_I}\ \underbrace{e^{iH_0t/\hbar}|\psi;t\rangle_S}_{|\psi;t\rangle_I}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}|\psi;t\rangle_I = V_I\,|\psi;t\rangle_I}$$

$\Rightarrow$ in Interaction Picture, state evolves ONLY with V_I !

Equally, for any time independent OPERATOR O

$$\frac{dO_I}{dt} = \frac{1}{i\hbar}[O_I, H_0]$$

~ Heisenberg Evolution with $H \to H_0$!

Now notice that we parametrized $|\psi;t\rangle_S$ as

$$|\psi;t\rangle_S = \sum_n c_n(t) e^{-iE_nt/\hbar} |n\rangle$$

$$\Downarrow$$

$$|\psi;t\rangle_I = \sum_n c_n(t) e^{-iE_nt/\hbar} e^{iH_0t/\hbar} |n\rangle$$

$$= \sum_n c_n(t) |n\rangle$$

same coefficients

$$\Rightarrow \langle m|\psi;t\rangle_I = \sum_n c_n(t) \underbrace{\langle m|n\rangle}_{\delta_{nm}}$$

$$c_n(t) = \langle n|\psi;t\rangle_I \; !$$

Use now diff. Eq. satisfied by $|\psi;t\rangle_I$ and contract by $\langle n|$

$$i\hbar \frac{\partial}{\partial t} \langle n|\psi;t\rangle_I = \langle n|V_I|\psi;t\rangle_I$$

$$= \sum_m \underbrace{\langle n|V_I|m\rangle} \langle m|\psi;t\rangle_I$$

$$\langle n|V_I|m\rangle = \langle n|e^{iH_0t/\hbar} V(t) e^{-iH_0t/\hbar}|m\rangle$$

$$= e^{i(E_n-E_m)t/\hbar} \underbrace{\langle n|V|m\rangle}_{V_{nm}(t)}$$

↳ we have

$$i\hbar \frac{\partial}{\partial t} c_n(t) = \sum_m V_{nm}(t)\, e^{i\underbrace{\frac{(E_n-E_m)}{\hbar}}_{\omega_{nm}}t} c_m(t)$$

$$= \sum_m V_{nm}(t)\, e^{i\omega_{nm}t} c_m(t)$$

$\Rightarrow$ to find time-dependence of some state $|\psi\rangle$, we need to solve system of linear coupled differential equations for $c_n(t)$, whose coefficients are matrix elements of the time-dependent potential !

Most of the times solving these equations exactly is IMPOSSIBLE and we need to resort to perturbation theory

Before going there, let's study a case where an EXACT SOLUTION is possible :

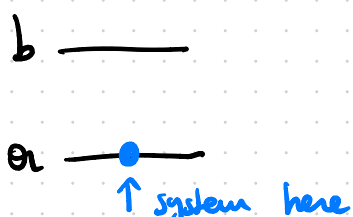
TWO-LEVEL SYSTEM

Consider a system that can be in two states & subject to an OSCILLATING POTENTIAL

While this seems now a "formal" problem, it can be used to model many important physical situations

- Atom in $\vec{E}(t)$ field that generates transitions among two states
- Spin Magnetic Resonance
- Masers etc...

two states $\{|a\rangle ; |b\rangle\}$ with $E_a ; E_b$ $E_b > E_a$



$$H_0 |a\rangle = E_a |a\rangle$$
$$H_0 |b\rangle = E_b |b\rangle$$

Unperturbed system

Using $|a\rangle, |b\rangle$ as basis

$$H_0 = E_a |a\rangle\langle a| + E_b |b\rangle\langle b| = \begin{bmatrix} E_a & 0 \\ 0 & E_b \end{bmatrix}$$

Now say $V(t)$ can generate transitions among the two states

$$V(t) = \gamma e^{i\omega t} |a\rangle\langle b| + \gamma e^{-i\omega t} |b\rangle\langle a|$$

$$= \begin{bmatrix} 0 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & 0 \end{bmatrix}$$

hermitian !

$\gamma \in \mathbb{R}$

Following our general formalism, we write for evolution of $|\psi\rangle_S$

$$|\psi, t\rangle_S = c_a(t) e^{-\frac{E_a t}{\hbar}} |a\rangle + c_b(t) e^{-iE_b t/\hbar} |b\rangle$$

$$i\hbar \frac{\partial}{\partial t} \begin{bmatrix} c_a(t) \\ c_b(t) \end{bmatrix} = \begin{bmatrix} 0 & \gamma e^{i\omega t} e^{i\omega_{ab} t} \\ \gamma e^{-i\omega t} e^{i\omega_{ba} t} & 0 \end{bmatrix} \begin{bmatrix} c_a(t) \\ c_b(t) \end{bmatrix}$$

$$\underline{\omega_{ba} = -\omega_{ab}} = \frac{E_b - E_a}{\hbar} > 0$$

$$i\hbar \frac{\partial}{\partial t}\begin{bmatrix} C_a(t) \\ C_b(t) \end{bmatrix} = \begin{bmatrix} 0 & \gamma e^{i\Delta t} \\ \gamma e^{-i\Delta t} & 0 \end{bmatrix} \begin{bmatrix} C_a(t) \\ C_b(t) \end{bmatrix}$$

$\Downarrow$

STANDARD first order system

with $\Delta = \omega_a - \omega_b + \omega$
$= \omega - \omega_{ba}$

solution can be obtained by deriving II ord eq. for one of the two, say for $C_a(t)$

$$\frac{d^2}{dt^2} C_a(t) - i\Delta \frac{dC_a(t)}{dt} + \frac{\gamma^2}{\hbar^2} C_a(t) = 0$$

searching for solutions as: $\underline{C_a(t) = e^{i\lambda t}}$ we get

$$\lambda^2 - \Delta\lambda - \frac{\gamma^2}{\hbar^2} = 0 \Rightarrow \lambda_\pm = \frac{\Delta}{2} \pm \underbrace{\sqrt{\frac{\Delta^2}{4} + \frac{\gamma^2}{\hbar^2}}}_{\Omega}$$

$$C_a(t) = A_+ e^{i\lambda_+ t} + A_- e^{i\lambda_- t}$$

boundary values !

and from system we have for $C_b(t)$

$$\gamma e^{i\Delta t} C_b(t) = i\hbar \frac{\partial}{\partial t} C_a(t)$$

$$= i\hbar \left[A_+ e^{i\lambda_+ t} i\lambda_+ + A_- e^{i\lambda_- t} i\lambda_- \right]$$

$$= -\hbar \lambda_+ A_+ e^{i\lambda_+ t} - \hbar \lambda_- A_- e^{i\lambda_- t}$$

$$C_b(t) = -\frac{\hbar \lambda_+}{\gamma} A_+ e^{-i\lambda_- t} - \frac{\hbar \lambda_-}{\gamma} A_- e^{-i\lambda_+ t}$$

now let's assume that $\left.\begin{array}{l} C_a(0) = 1 \\ C_b(0) = 0 \end{array}\right\}$ Boundaries

$\Rightarrow$ system starts @ $t=0$ in $|a\rangle$, then:

$$C_a(0) = A_+ + A_- = 1$$

$$C_b(0) = -\frac{\cancel{\hbar} \lambda_+ A_+}{\cancel{\gamma}} - \frac{\cancel{\hbar} \lambda_- A_-}{\cancel{\gamma}} = 0$$

$$\Rightarrow \begin{cases} A_+ + A_- = 1 \\ \lambda_+ A_+ + \lambda_- A_- = 0 \end{cases} \Rightarrow \begin{aligned} A_+ &= -\frac{\lambda_-}{\lambda_+ - \lambda_-} \\ A_- &= +\frac{\lambda_+}{\lambda_+ - \lambda_-} \end{aligned}$$

$$A_+ = -\frac{\lambda_-}{2\Omega} \qquad A_- = \frac{\lambda_+}{2\Omega}$$

$$C_a(t) = \frac{1}{2\Omega}\left[\lambda_+ e^{i\lambda_- t} - \lambda_- e^{i\lambda_+ t}\right]$$

$$C_b(t) = -\frac{\hbar}{2\gamma}\frac{\lambda_+\lambda_-}{\Omega}\left[e^{-i\lambda_+ t} - e^{-i\lambda_- t}\right]$$

$$= -\frac{\hbar}{2\gamma}\frac{\lambda_+\lambda_-}{\Omega} e^{-i\frac{\Delta}{2}t}\left[e^{-i\Omega t} - e^{+i\Omega t}\right]$$

$$c_b(t) = 2i \frac{\hbar}{2\gamma} \frac{\lambda_+\lambda_-}{\Omega} e^{-i\frac{\Delta}{2}t} \sin \Omega t$$

which gives for the probability of finding

$|\psi;t\rangle$ in $|b\rangle$ @ time t

$$P_b(t) = |c_b(t)|^2 = \frac{\hbar^2}{\gamma^2}\left[\frac{\gamma^4}{\hbar^4}\right]\frac{1}{\left[\frac{\Delta^2}{4}+\frac{\gamma^2}{\hbar^2}\right]} \sin^2(\Omega t)$$

$$= \frac{\gamma^2/\hbar^2}{\gamma^2/\hbar^2 + \frac{(\omega-\omega_{ba})^2}{4}} \sin^2(\Omega t)$$

RABI FORMULA

and $|c_a(t)|^2 = 1 - |c_b(t)|^2$

Probability oscillates with typical frequency

$$\Omega = \sqrt{\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{ba})^2}{4}}$$

RABI FREQUENCY

RESONANCE CONDITION

if angular frequency of potential $\omega \sim \omega_{ba} = \frac{E_b - E_a}{\hbar}$

then $\Omega \sim \frac{\gamma}{\hbar}$

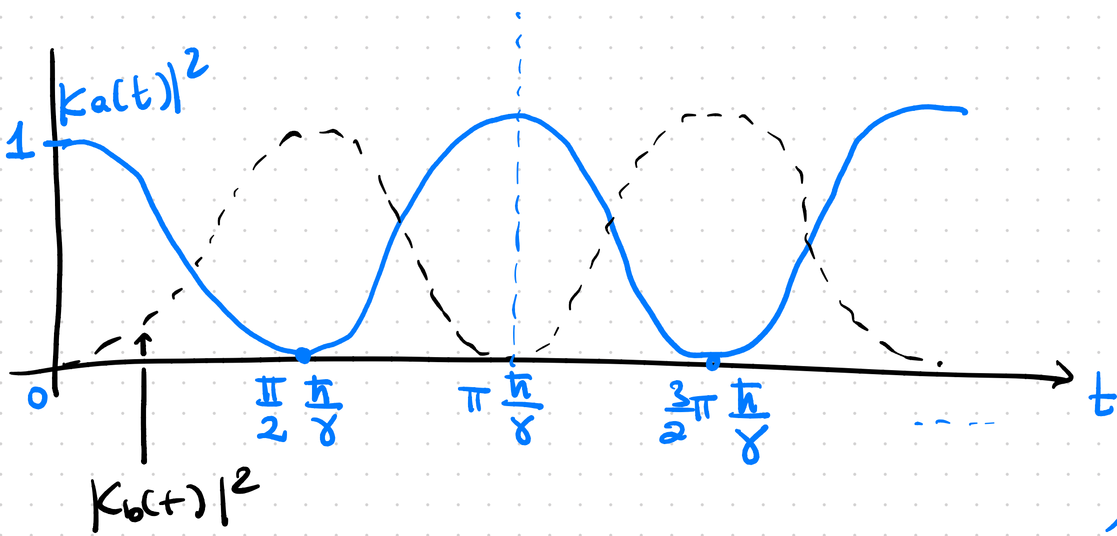
remember

$$\left[\begin{array}{l} \Omega = \sqrt{\frac{\Delta^2}{4} + \frac{\gamma^2}{\hbar^2}} \\ \Delta = \omega - \omega_{ba} \end{array}\right]$$

$$|c_b(t)|^2 \sim \sin^2\left[\frac{\gamma}{\hbar} t\right]$$

amplitude of oscillation reaches 1

this is called **RESONANCE**

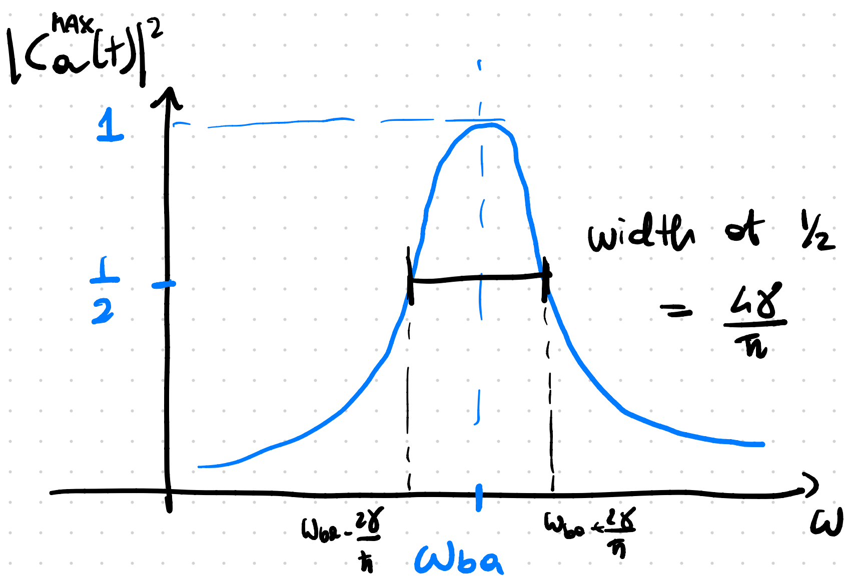


from $t=0$ to $t = \frac{\pi}{2}\frac{\hbar}{\gamma}$, the system absorbs energy from the potential and goes from $E_a \to E_b$

then from $t = \frac{\pi}{2}\frac{\hbar}{2} \to t = \pi\frac{\hbar}{\gamma}$ energy goes back into potential and system returns to original state

PERIOD $T = \pi \frac{\hbar}{\gamma} = \frac{\pi}{\Omega}$ due to $\sin^2$

of course, away from resonance $|c_a(t)|^2 < 1$



↑ resonance frequency

$\gamma \to 0$ WEAK POTENTIAL

$\Rightarrow$ NARROWER PEAK !

these two-state systems have various applications

- Atoms in $\vec{E}$ field $\Rightarrow$ we will discuss more about this later in the course
- Spin Magnetic Resonance
- Masers
- . . . .

SPIN - MAGNETIC RESONANCE

At the basis of MRI systems in Hospitals

Consider a spin $\frac{1}{2}$ system (ELECTRON) bound in an Atom (typically Hydrogen)

Apply $\vec{B} = B_0 \hat{z} + B_1 (\hat{x} \cos \omega t + \hat{y} \sin \omega t)$

constant along z rotating in (x, y)

In previous picture, here $B_0 \hat{z} = H_0$

$B_1[\dots] = V(t)$

Electron magnetic moment $\vec{\mu} = \frac{e}{mc}\vec{S}$

so that $H = -\frac{e}{mc}\bar{S}\cdot\bar{B}$ and therefore explicitly

$$H_0 = -\frac{eB_0}{mc} S_z$$

$$V(t) = -\frac{eB_1}{mc}\left[\cos\omega t\, S_x + \sin\omega t\, S_y\right]$$

Use now $S_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle$ to write

$$S_z = \frac{\hbar}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right)$$

$$S_x = \frac{\hbar}{2}\left(|+\rangle\langle-| + |-\rangle\langle+|\right)$$

$$S_y = i\frac{\hbar}{2}\left(|-\rangle\langle+| - |+\rangle\langle-|\right)$$

An obvious way to check these is verifying that

$$[S_i, S_j] = i \varepsilon_{ijk} \hbar S_k$$ commutation relations

For e^- $e<0$ and

$$H_0 |+\rangle = E_+ |+\rangle \qquad E_+ = \frac{|e|\hbar B_0}{2mc}$$

$$H_0 |-\rangle = E_- |-\rangle \qquad E_- = -\frac{|e|\hbar B_0}{2mc}$$

$E_+ > E_-$

$E_+ \downarrow$ level "b"

$E_- \searrow$ level "a"

then $$\omega_{ba} = \frac{E_+ - E_-}{\hbar} = \frac{|e| B_0}{mc}$$ "resonance" frequency

$\Rightarrow$ if $B_1 = 0$, then this is PRECESSION frequency for e^- spin in constant $\vec{B}_z$ field!

As long as $B_1 = 0$, the probabilities of being in state $|+\rangle$ or $|-\rangle$ don't change, DESPITE SPIN PRECESSION

$$|\psi;t\rangle_{B_1=0} = C_+(t)|+\rangle + C_-(t)|-\rangle$$

$|C_+|^2$ & $|C_-|^2$ constant

with $B_1 \neq 0$, comparing with general formulas

$$V(t) = +\frac{|e|\hbar B_1}{2mc}\Big[|+\rangle\langle -|\left(\cos\omega t - i\sin\omega t\right)$$

$$+ |-\rangle\langle +|\left(\cos\omega t + i\sin\omega t\right)\Big]$$

$$= \frac{|e|\hbar B_1}{2mc}\Big[e^{-i\omega t}\underset{b}{|+\rangle}\underset{a}{\langle -|} + e^{i\omega t}\underset{a}{|-\rangle}\underset{b}{\langle +|}\Big]$$

so we can identify $\gamma = \frac{|e| \hbar B_1}{2mc}$

At resonance $\left[\omega = \omega_{ba} = \frac{|e| B_0}{mc} \right]$

spin flips $|+\rangle \leftrightarrow |-\rangle$ in addition to

precession generated by $B_0 \hat{z}$

RESONANCE can be obtained adjusting frequency of rotating field to match precession frequency

$\Rightarrow$ in this way, by varying frequency of rotating field one can precisely measure magnetic moment μ

MRI works detecting radio frequency induced by spin polarization evolution during time !

Finally notice that in practice rotating fields are difficult to produce. Same effect can be obtained with oscillating fields in $\hat{x}$ or $\hat{y}$ direction; for example

$$B_1 \hat{x} \cos \omega_x t \equiv \frac{B_1}{2}\left[\hat{x}\cos\omega t + \hat{y}\sin\omega t\right] \} f_{cc}$$

$$+ \frac{B_1}{2}\left[\hat{x}\cos\omega t - \hat{y}\sin\omega t\right] \} f_c$$

$$\underset{\text{counterclockwise}}{f_{cc}(\omega)} = \underset{\text{clockwise}}{f_c(-\omega)}$$

get effect of f_c sending $\underline{\omega \to -\omega}$ in previous formulas

if we get RESONANCE on one of the two, the other is negligible if

$$B_1 \ll B_0 \implies \frac{\gamma}{\hbar} \ll \omega_{ba}$$