

Advanced Quantum Mechanics

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Quantum Dynamics

Lecture #3

Recap of Last Class

- Time Dependent Perturbation Theory
- Linear Response Function and Spectral Decomposition
- Real and Imaginary Part of Response Fn.
- Fermi's Golden Rule and Transition Probabilities

Quantum Adiabatic Theorem

Consider a **time dependent Hamiltonian** $H(t)$. If H was time independent, we have seen that expanding the state of the system in this basis simplifies the dynamics.

Is it useful to expand the state in the **eigenbasis of the instantaneous Hamiltonian $H(t)$** for each time-point t ? This would in general be **a time-dependent basis set**, since Hamiltonians at different time points do not commute.

Quantum Adiabatic Theorem (Max Born and Vladimir Fock, 1928)

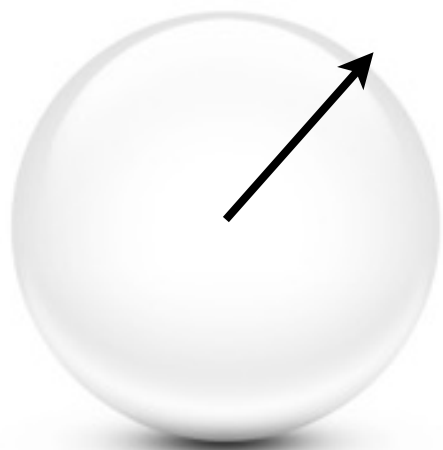
For a continuously evolving of Hamiltonian, **whose changes are slow enough**, a quantum system, which is **initially in the eigenstate of the instantaneous Hamiltonian**, **follows this state** provided **the eigenvalue of this state is nondegenerate and separated from the rest of the (instantaneous) Hamiltonian's spectrum at all times**.

Quantum Adiabatic Theorem

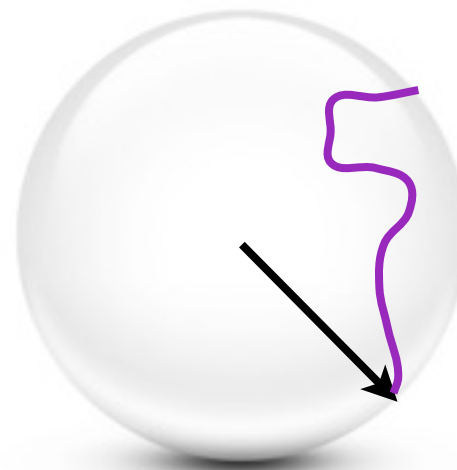
A spin 1/2 object in a magnetic field. 2D Hilbert space with a Hamiltonian

$$H(t) = -\mu_B \vec{B}(t) \cdot \vec{\sigma}$$

Assume that magnitude of the magnetic field is fixed, while its direction varies with time.



$\hat{n}(0)$



$\hat{n}(t)$

Define the basis states

$$|\hat{n}, +\rangle \quad \text{and} \quad |\hat{n}, -\rangle$$

$$\text{where } \vec{\sigma} \cdot \hat{n} |\hat{n}, \pm\rangle = \pm \frac{1}{2} |\hat{n}, \pm\rangle$$

$$\text{If } \vec{B}(t) = B \hat{n}(t) \quad |\hat{n}(t), \pm\rangle$$

is the basis where the instantaneous Hamiltonian $H(t)$ is diagonalized

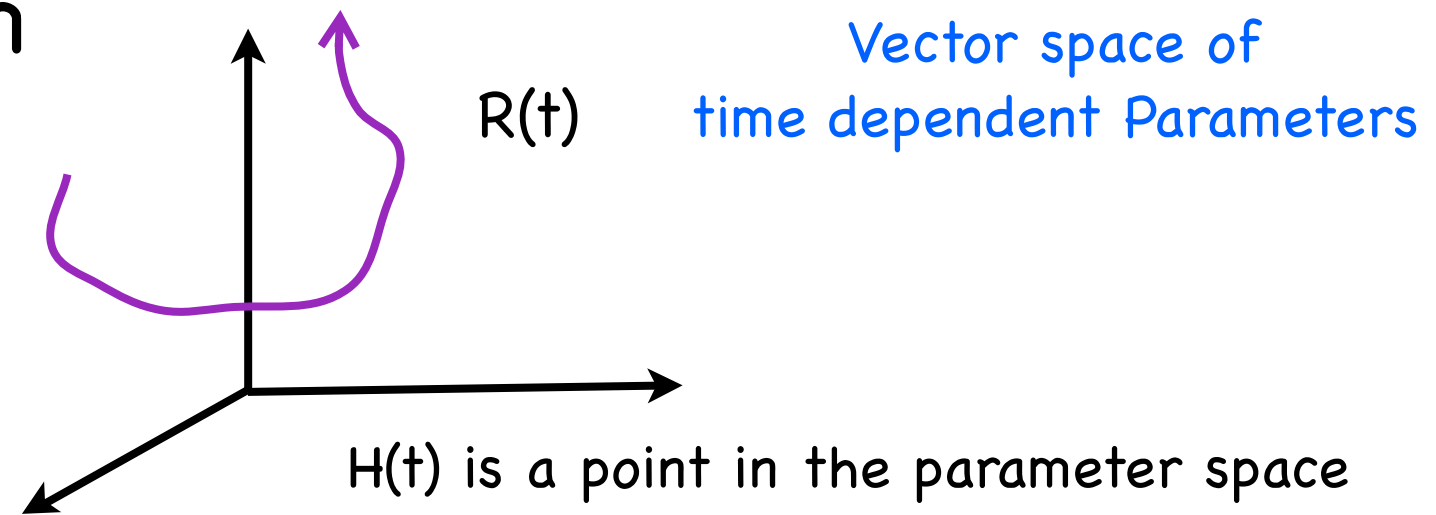
The eigenvalues of the instantaneous Hamiltonian : $\mp \frac{1}{2} \mu_B B$ gapped spectrum at all times

The Quantum Adiabatic theorem, in this case, states that, if we start the system in the state $|\hat{n}(0), +\rangle$, the system will evolve to $|\hat{n}(t), +\rangle$. Similarly, if we start with $|\hat{n}(0), -\rangle$, the system will evolve to $|\hat{n}(t), -\rangle$

Quantum Adiabatic Theorem

- $i\partial_t|\psi(t)\rangle = \hat{H}[R(t)]|\psi(t)\rangle$

The Hamiltonian at time t is completely specified by the values of (possibly >1) parameters which change with time.



As the parameters change in time, one traces out a curve in the parameter space, $R(t)$

Correspondingly, at each time (or for each R), there is a basis which diagonalizes $H[R(t)]$

- $\hat{H}[R(t)]|n[R(t)]\rangle = \epsilon_n[R(t)]|n[R(t)]\rangle$

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-i \int_0^t dt' \epsilon_n(t')} |n(t)\rangle = \sum_n c_n(t) e^{-i\theta_n(t)} |n(t)\rangle$$

From ●

$$\sum_n [\epsilon_n c_n(t) + i\dot{c}_n(t)] e^{-i\theta_n(t)} |n(t)\rangle + i c_n(t) e^{-i\theta_n(t)} |\dot{n}(t)\rangle = \sum_n c_n(t) \epsilon_n(t) e^{-i\theta_n(t)} |n(t)\rangle$$

Using $\langle m(t)|n(t)\rangle = \delta_{mn}$ $\dot{c}_m(t) = -c_m(t) \langle m|\dot{n}\rangle - \sum_{n \neq m} c_n(t) e^{i[\theta_m(t) - \theta_n(t)]} \langle m|\dot{n}\rangle$

Quantum Adiabatic Theorem

$$\hat{H}(t)|n(t)\rangle = \epsilon_n(t)|n(t)\rangle$$

Taking time derivative

$$\dot{\hat{H}}(t)|n(t)\rangle + \hat{H}(t)|\dot{n}(t)\rangle = \dot{\epsilon}_n(t)|n(t)\rangle + \epsilon_n(t)|\dot{n}(t)\rangle$$

$$\dot{\epsilon}_n(t)\delta_{mn} + \epsilon_n(t)\langle m(t)|\dot{n}(t)\rangle = \langle m(t)|\dot{\hat{H}}(t)|n(t)\rangle + \langle m(t)|\hat{H}(t)|\dot{n}(t)\rangle$$

$$\epsilon_m(t)\langle m(t)|\dot{n}(t)\rangle$$

So $\langle m(t)|\dot{n}(t)\rangle = \frac{\langle m(t)|\dot{\hat{H}}(t)|n(t)\rangle}{\epsilon_n(t) - \epsilon_m(t)}$ for $m \neq n$

$$\dot{c}_m(t) = -c_m(t)\langle m(t)|\dot{n}(t)\rangle - \sum_{n \neq m} c_n(t)e^{i[\theta_m(t) - \theta_n(t)]} \frac{\langle m(t)|\dot{\hat{H}}(t)|n(t)\rangle}{\epsilon_n(t) - \epsilon_m(t)}$$

Adiabaticity condition is equivalent to neglecting the second term on RHS

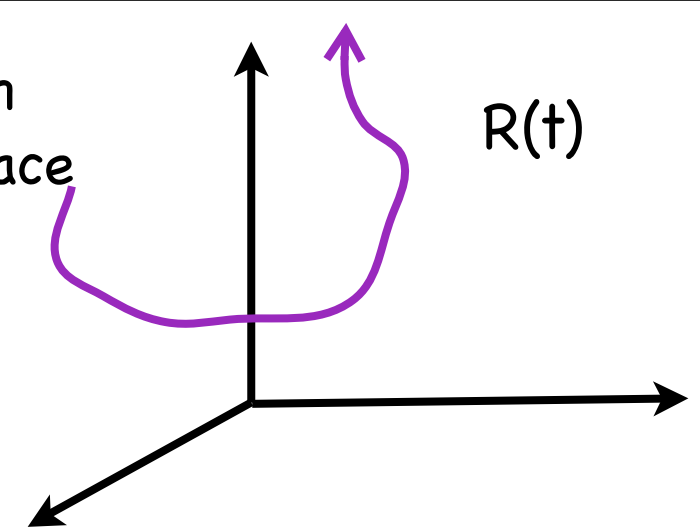
$$\sum_n |c_n(t)|^2 = 1 \Rightarrow |c_n(t)| < 1 \quad \text{Adiabaticity condition} \quad \langle m|\dot{\hat{H}}|n\rangle \ll (\epsilon_n - \epsilon_m)\langle m|\dot{n}\rangle$$

For lowest energy gap

$$\Delta = \text{Min}(\epsilon_n - \epsilon_m)$$

$$\langle m|\dot{\hat{H}}|n\rangle \ll \Delta\langle m|\dot{n}\rangle$$

$H(t)$ is a point in the parameter space



Vector space of time dependent Parameters

Berry Phase

For adiabatic processes, starting from a non-degenerate state

$$c_m(t) = c_m(0)e^{-\int_0^t dt' \langle m(t') | \dot{m}(t') \rangle} = c_m(0)e^{i\gamma_m}$$

Berry's Phase $\gamma_m(t) = i \int_0^t dt' \langle m(t') | \dot{m}(t') \rangle$

- Extra phase due to time-dependent basis
- Separate from the dynamic phase θ_m

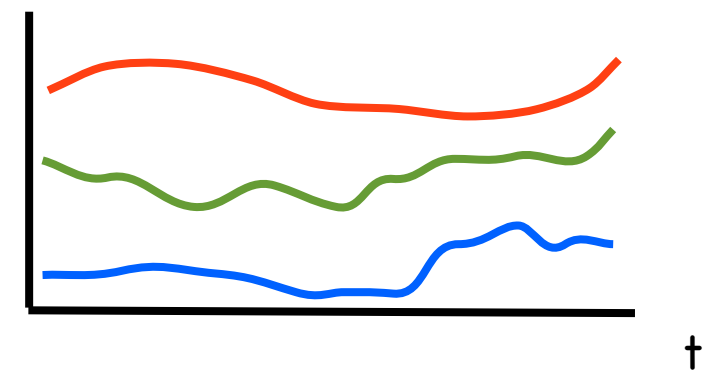
Starting from an eigenstate of the initial Hamiltonian

$$c_m(0) = 1 \text{ for } m = m_0$$

$$c_m(0) = 0 \text{ for } m \neq m_0$$

$$|\psi_n(t_f)\rangle = e^{i(\theta_n + \gamma_n)} |\psi(0)\rangle$$

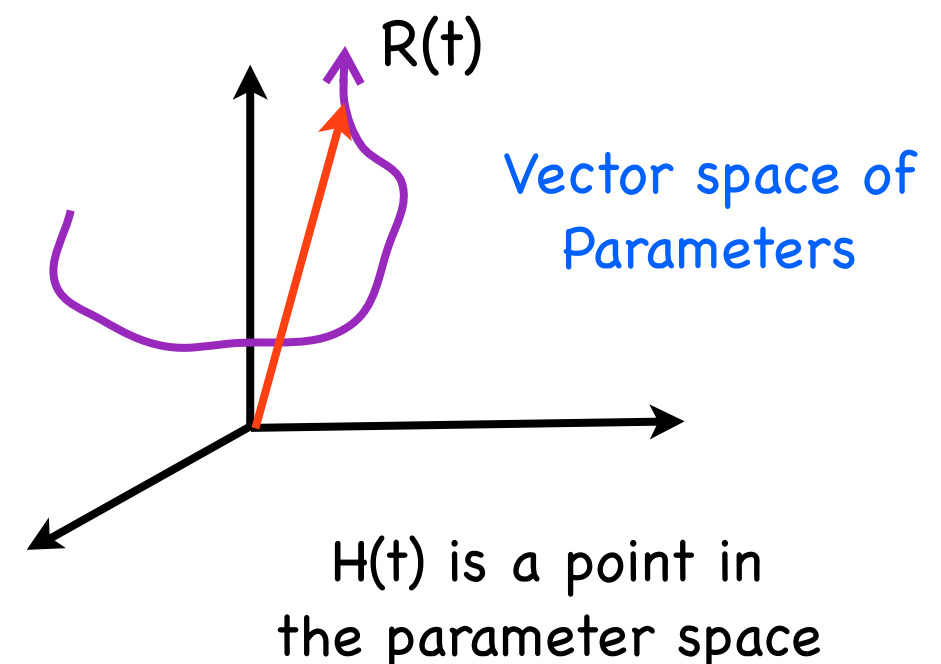
The system remains in the corresponding instantaneous eigenstate



$$\gamma_n(t) = i \int_0^{t_f} dt' \langle n[R(t')] | \dot{n}[R(t')] \rangle = i \int_0^{t_f} dt' \dot{R} \langle n[R(t')] | \nabla_R | n[R(t')] \rangle$$

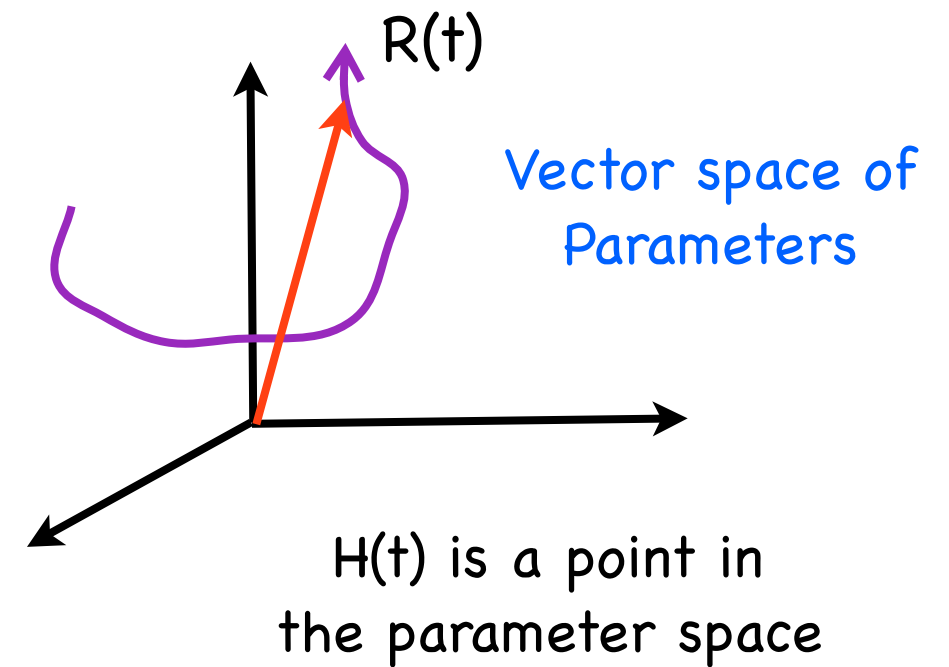
$$= \int \vec{A}(\vec{R}) \cdot d\vec{R}$$

Vector Potential/Berry Connection $\vec{A}(R) = i \langle n(R) | \nabla_R | n(R) \rangle$



Berry Phases and Gauge Invariance

At each point in the trajectory, the instantaneous Hamiltonian specifies the eigenbasis upto an overall phase which we can choose. This is a position (in the param space) dependent phase rotation (a U(1) gauge symmetry).



Let us assume we can choose the phase of the state we are tracking. All other phases are fixed by $H[R(t)]$.

$$|n(R)\rangle \rightarrow e^{i\phi(R)} |n(R)\rangle \quad \vec{A}(R) = i\langle n(R) | \nabla_R | n(R) \rangle \rightarrow i\langle n(R) | e^{-i\phi(R)} \nabla_R e^{i\phi(R)} | n(R) \rangle$$

$$= i\langle n(R) | \nabla_R | n(R) \rangle - \nabla_R \phi(R) = \vec{A}(R) - \nabla_R \phi(R)$$

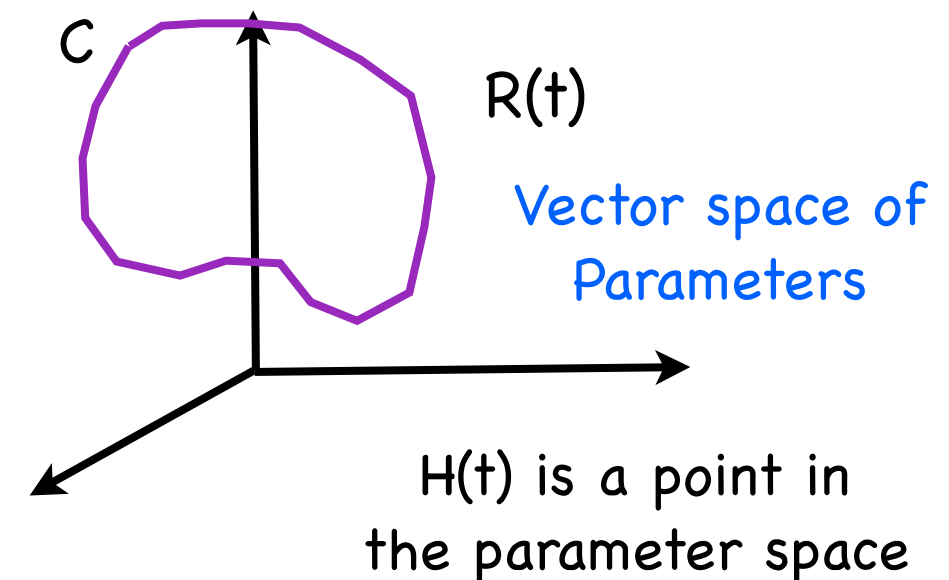
Berry potential is not a gauge invariant quantity

Berry, 1973: Consider the evolution on a closed path, so that $H(T)=H(0)$.

Berry phase for this evolution

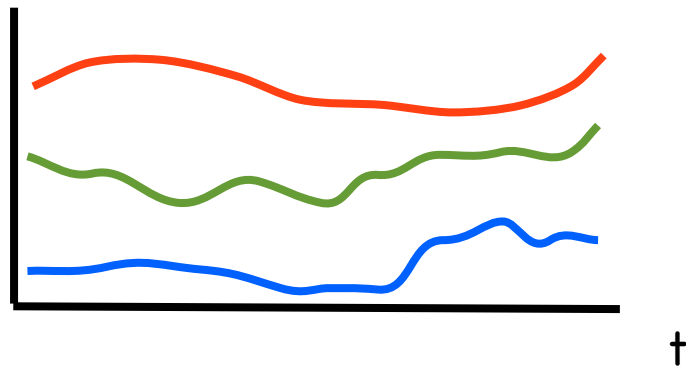
$$\gamma_n(C) = \oint_C \vec{A}(R) \cdot dR$$

is a gauge invariant quantity

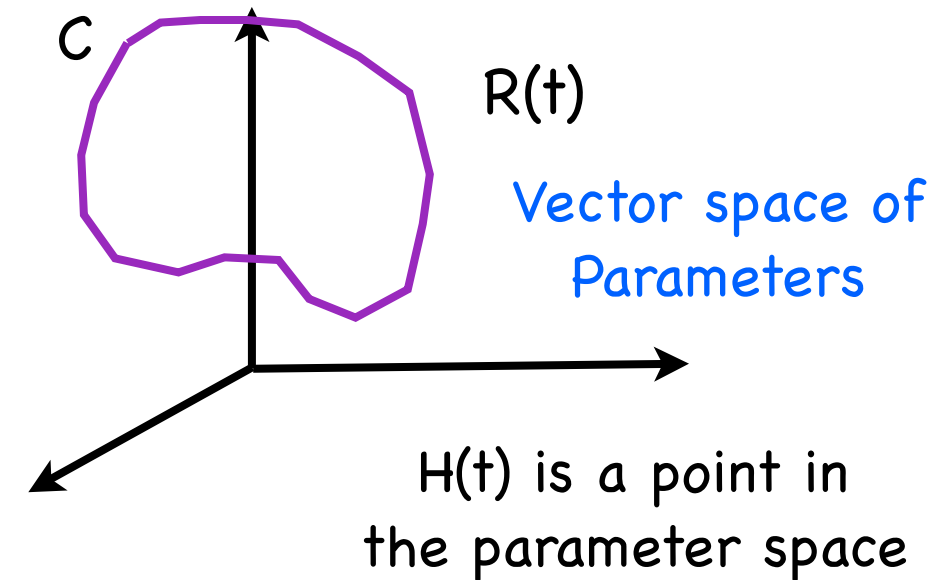


Berry Phase for closed paths

What happens to the system if we adiabatically take it along a closed path?



The system remains in the corresponding instantaneous eigenstate



$$|\psi_n(t_f)\rangle = e^{i(\theta_n + \gamma_n)} |\psi(0)\rangle$$

Dynamic Phase

depends on how fast or slow the circuit C is traversed.

Geometric or Berry Phase

depends on the circuit C, but not on how it is traversed in time

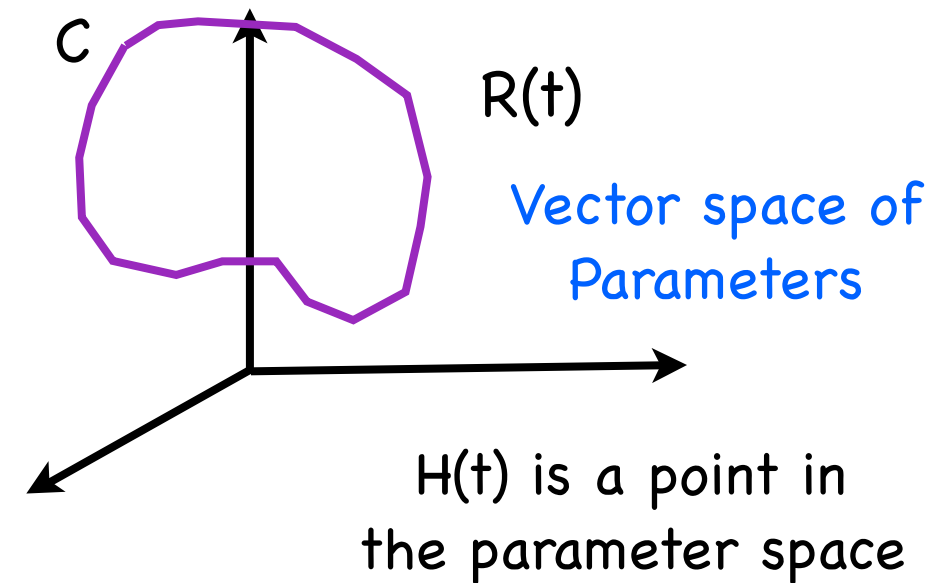
Berry Curvature

Consider 3-dimensional space of parameters, and use Stokes Theorem

$$\gamma_n(C) = i \int \int_C d\vec{S} \cdot \nabla \times \langle n[R] | \nabla_R n[R] \rangle = -Im \int \int_C \langle \nabla_R n[R] | \times | \nabla_R n[R] \rangle$$

$$= -Im \sum_{m \neq n} \int \int_C d\vec{S} \cdot \langle \nabla_R n[R] | m \rangle \times \langle m | \nabla_R n[R] \rangle$$

where S is any surface
which has C as its boundary



Use $\langle m | \nabla n \rangle = \frac{\langle m | \nabla \hat{H} | n \rangle}{\epsilon_n - \epsilon_m}$ to write $\gamma_n(C) = - \int \int_C d\vec{S} \cdot \vec{B}_n(R)$

$$\vec{B}_n(R) = Im \sum_{m \neq n} \frac{\langle n(R) | \nabla_R \hat{H}(R) | m(R) \rangle \times \langle m(R) | \nabla_R \hat{H}(R) | n(R) \rangle}{(E_n(R) - E_m(R))^2}$$

Effective Magnetic
Field/ Berry Curvature

The Berry curvature is a gauge invariant quantity

Degeneracy Points and Simplification

Berry phase calculation simplifies for trajectories near a degeneracy point (which avoid this degenerate point).

$$\gamma_n(C) = - \int \int_C d\vec{S} \cdot \vec{B}_n(R) \quad \vec{B}_n(R) = \text{Im} \sum_{m \neq n} \frac{\langle n(R) | \nabla_R \hat{H}(R) | m(R) \rangle \times \langle m(R) | \nabla_R \hat{H}(R) | n(R) \rangle}{(E_n(R) - E_m(R))^2}$$

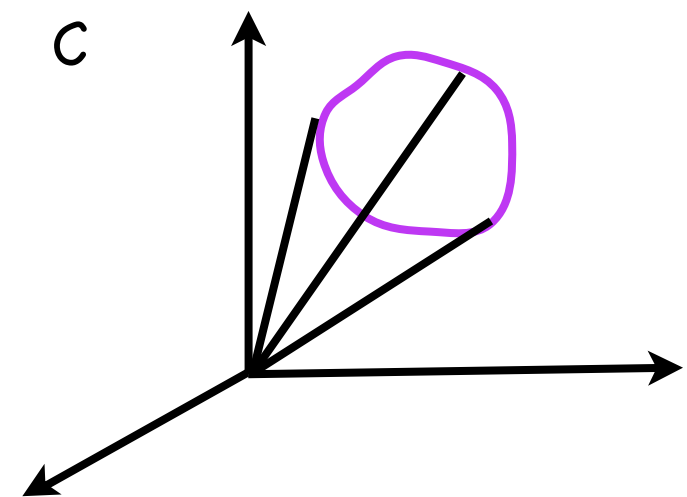
Simplest Case: A degeneracy of 2 states ($|+\rangle$ and $|-\rangle$) at $R=R_0$. **Ignore other states:** finite energy denominator $\rightarrow$ Work with 2X2 Hamiltonian in this space.

Most General 2X2 Hamiltonian $H(R) = \frac{1}{2} \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & -H_z \end{pmatrix} = \frac{1}{2} \vec{R} \cdot \vec{\sigma} \quad \vec{R} = (H_x, H_y, H_z)$

$$\nabla_R H = \frac{1}{2} \vec{\sigma} \quad E_{\pm}(\vec{R}) = \pm R \quad \text{Use all your expertise with spin-1/2 objects to get}$$

$$\vec{B}_{\pm}(\vec{R}) = \pm \frac{\vec{R}}{R^3} \quad \gamma_{\pm}(C) = \mp \frac{1}{2} \Omega_C$$

Ω_C is the solid angle subtended by the circuit C at the degeneracy point.

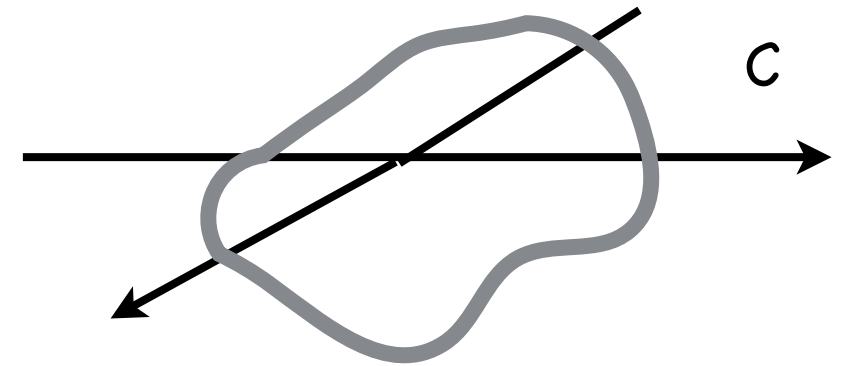


Topological Invariants

For a 2 state system with time varying Hamiltonian, the Berry phase is given by

$$\gamma_{\pm}(C) = \mp \frac{1}{2} \Omega_C \quad \Omega_C \text{ is the solid angle subtended by the circuit } C \text{ at the degeneracy point.}$$

Now consider a 2D parameter space, say H_y is 0



If H_y is 0, $\exp[i \gamma(C)] = -1$ if C encloses degeneracy point and $\exp[i \gamma(C)] = 1$ if it does not.

$\gamma(C) = \pi$ if C encloses degeneracy point and $\gamma(C) = 0$ if it does not.

The Berry phase is topological in the sense that contours that can be smoothly deformed to each other have the same Berry phase.

The degeneracy point acts as a “puncture” in this manifold and loops enclosing this point have a different topology than those not enclosing it.

State Systems and Rabi Oscillation

2-state system with time indep. Hamiltonian

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$$

Harmonic time-dependent off-diagonal term

$$H_1(t) = \Omega(e^{i\omega t} + e^{-i\omega t})|1\rangle\langle 2| + h.c.$$

Example: Two level atom interacting with classical radiation field.



Transform to a time dependent basis, which rotates in time with the freq of the pert.

$$|1'\rangle = e^{i\omega t}|1\rangle \quad |2'\rangle = |2\rangle$$

This is different from going to interaction representation.

There, states rotate with their unperturbed energies as freq. Here the rotation freq. is the perturbation frequency. However, at resonance ($\omega = E_2 - E_1$), the two approaches are exactly same.

2 State Systems and Rabi Oscillation

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$$

$$H_1(t) = \Omega(e^{i\omega t} + e^{-i\omega t})|1\rangle\langle 2| + h.c.$$

Example: Two level atom interacting with classical radiation field.



In the rotating basis: $|1'\rangle = e^{i\omega t}|1\rangle$ $|2'\rangle = |2\rangle$

$$H = E_1|1'\rangle\langle 1'| + E_2|2'\rangle\langle 2'| + \Omega[|1'\rangle\langle 2'| + |2'\rangle\langle 1'|]$$

~~$$+ \Omega[e^{-2i\omega t}|1'\rangle\langle 2'| + e^{2i\omega t}|2'\rangle\langle 1'|]$$~~

RWA

Rotating Wave Approximation:

In the basis rotating with the perturbation, terms with explicit dynamics on the scale of the perturbation freq. are neglected (set to 0 by hand). Implicit assumption: we (the measurement process) averages over timescales much larger than ω^{-1} .

RWA and Dressed States

$$|\psi(t)\rangle = c_1(t)|1'\rangle + c_2(t)|2'\rangle$$

Schrodinger Equation:
(Time Dep. Basis)

$$i \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \end{pmatrix} = \begin{pmatrix} E_1 + \omega & \Omega \\ \Omega & E_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Initial Condition:

$$c_1(0) = 1, \quad c_2(0) = 0$$

Dressed Hamiltonian

Rabi Frequency

Eigenvalues: $E^\pm = \frac{E_1 + E_2 + \omega}{2} \pm \sqrt{\frac{(E_2 - E_1 - \omega)^2}{4} + \Omega^2}$ $\omega_R = \sqrt{\frac{(\omega - E_{21})^2}{4} + \Omega^2}$

Eigenstates: $|\psi^{+(-)}\rangle = \begin{pmatrix} u(-v) \\ v(u) \end{pmatrix}$ $u^2 = 1 - v^2 = \frac{1}{2} \left[1 + \frac{\omega - E_{21}}{2\sqrt{(\omega - E_{21})^2/4 + \Omega^2}} \right]$

Dressed States: Eigenstates of the "Hamiltonian" in the rotating basis

Transform back to get dynamics

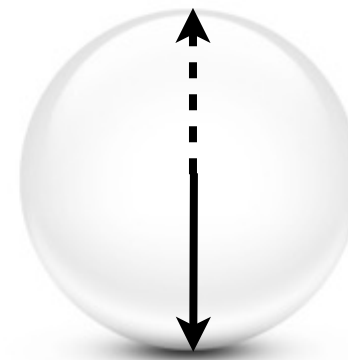
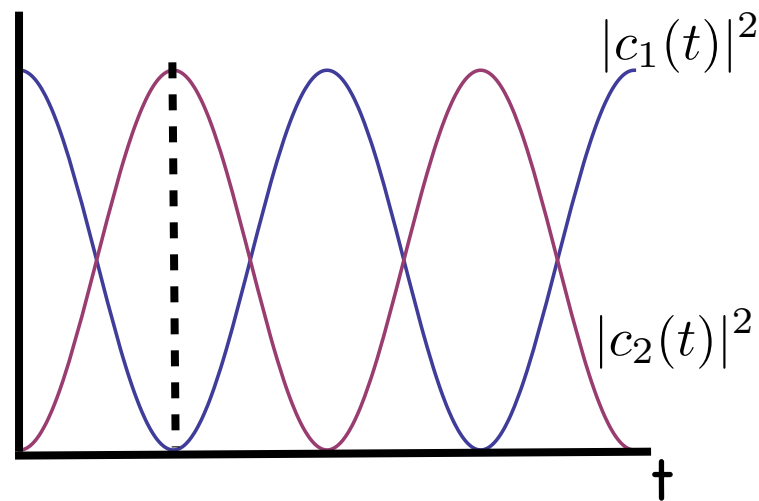
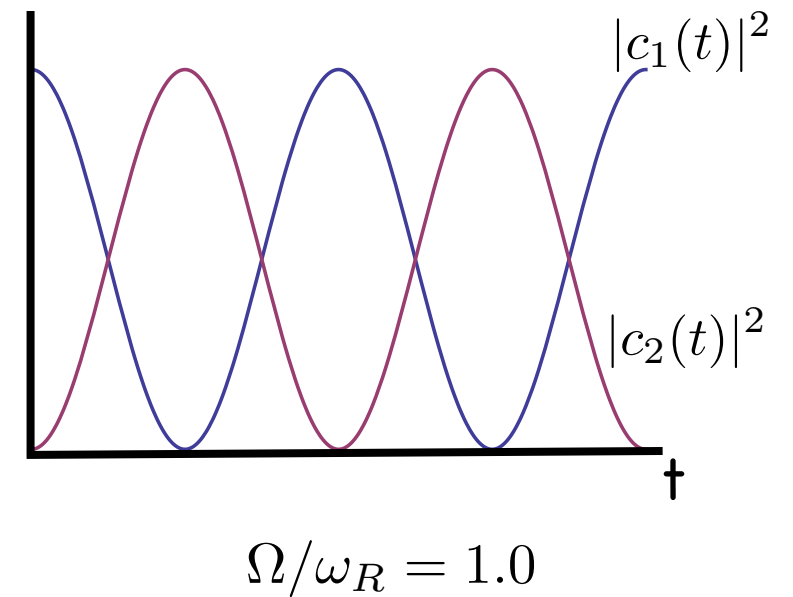
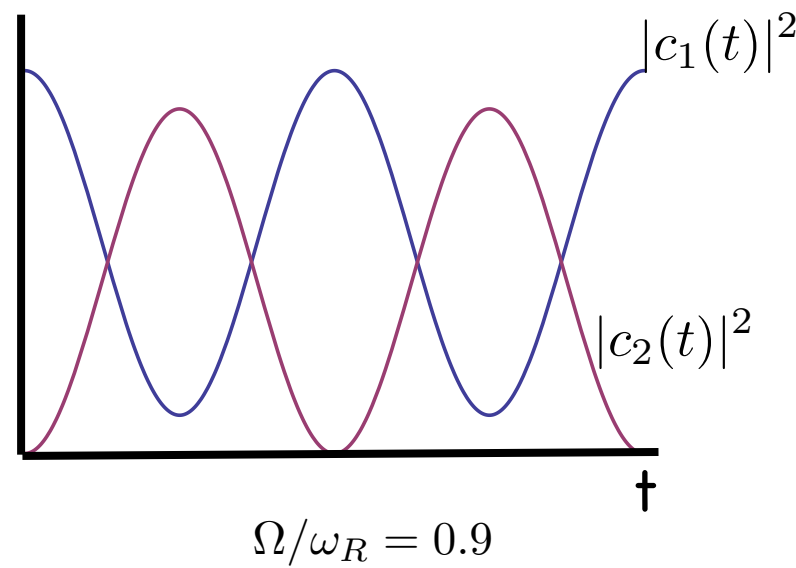
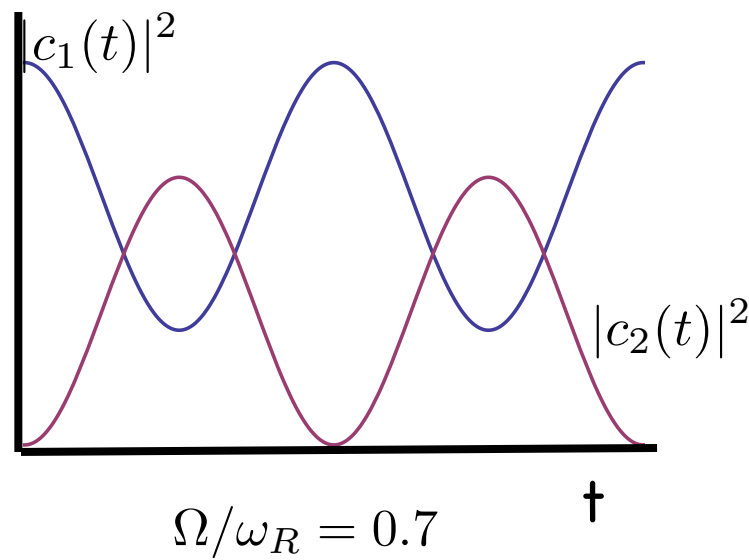
$$c_1(t) = u^2 e^{-iE^+ t} + v^2 e^{-iE^- t}$$

$$c_2(t) = uv[e^{-iE^+ t} - e^{-iE^- t}]$$

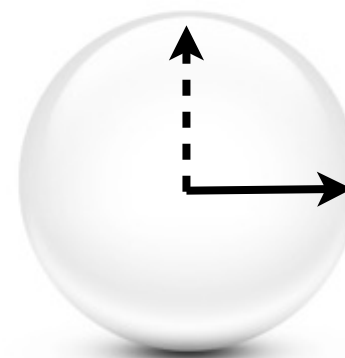
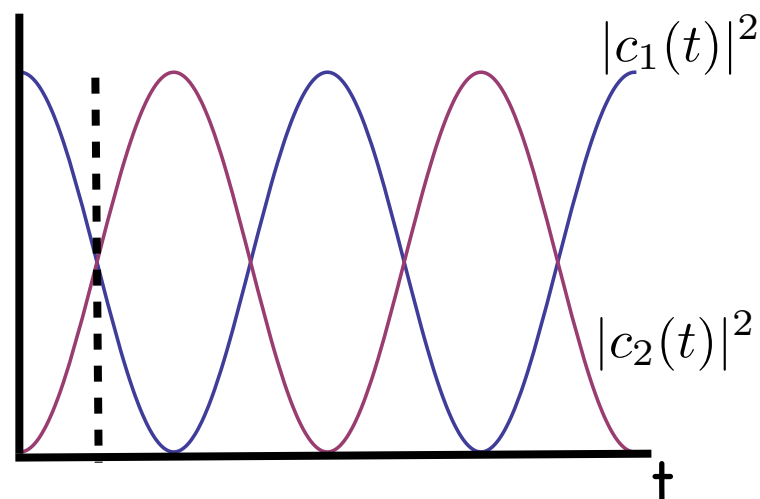
So, $|c_1(t)|^2 = 1 - \frac{\Omega^2}{\omega_R^2} \sin^2(\omega_R t)$ $|c_2(t)|^2 = \frac{\Omega^2}{\omega_R^2} \sin^2(\omega_R t)$

2 State Systems and Rabi Oscillation

Rabi Frequency $\omega_R = \sqrt{\frac{(\omega - E_{21})^2}{4} + \Omega^2}$

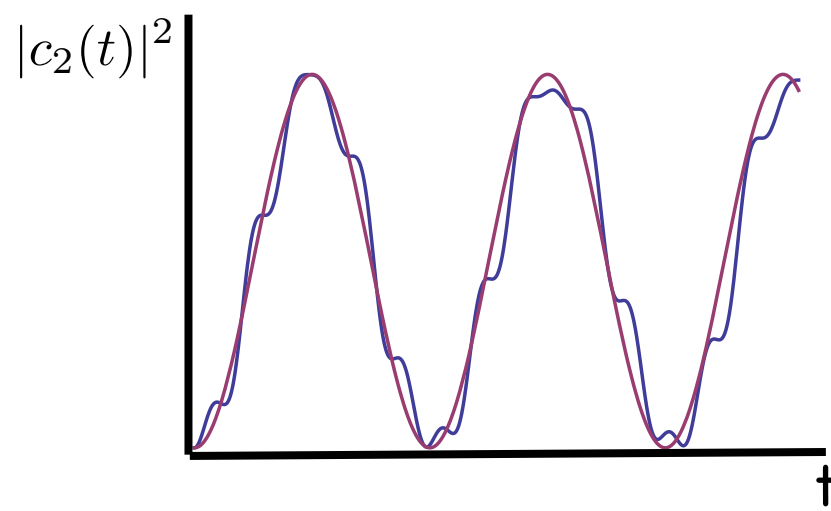
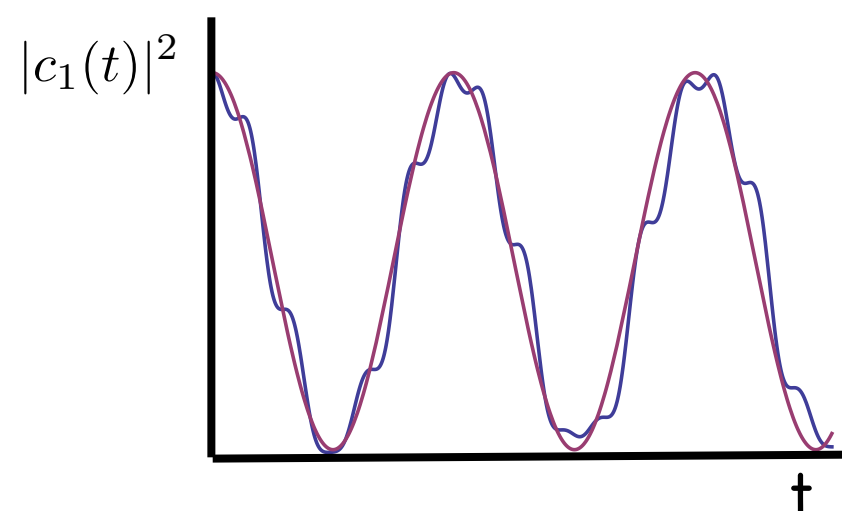


π Pulse: Population in $S_z = -1/2$ state



$\pi/2$ Pulse: Population in S_y state

Rabi Oscillations and RWA



RWA vs. Full
Numerical Solution

RWA misses
the fast wiggles

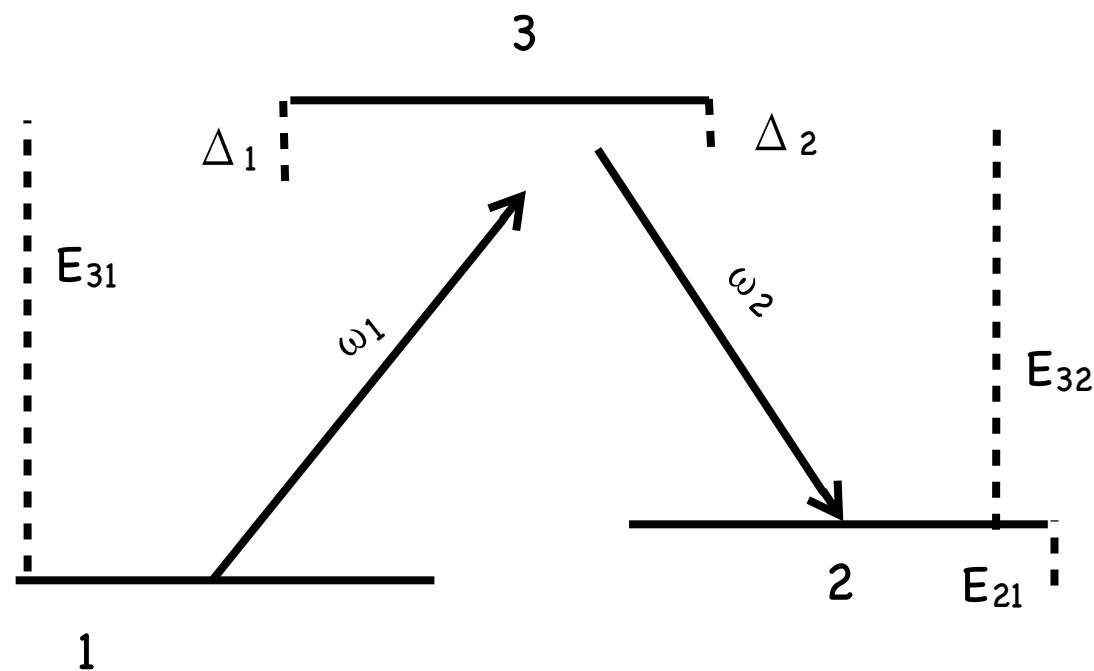
As the frequency of the perturbation nears resonance, i.e. for $\omega - E_{21} \ll \Omega$

$\omega_R \sim \Omega + \frac{(\omega - E_{21})^2}{8\Omega^2}$ the transition probability oscillates with time with the Rabi frequency.

- ☑ Quite different from linear response theory (where osc. are at driving frequency ω) or from Fermi golden rule where transition probability scales with time.
- ☑ Notice that we have not talked about “weak” or perturbative drive. In fact, near resonance, the coupling of the time dependent part dominates the whole action.
- ☑ This type of drive is often called coherent coupling of states/coherent drives, since the drive induces phase correlations between the 2 states.

Near resonance we do have a small parameter Δ/Ω , where Δ is the detuning from the transition. This is a question of having different time-scales in the problem.

RWA with 3 states



Three state system and 2 optical perturbation

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| + E_3|3\rangle\langle 3|$$

$$H_1(t) = \Omega_1(e^{i\omega_1 t} + e^{-i\omega_1 t})|1\rangle\langle 3| + \Omega_2(e^{i\omega_2 t} + e^{-i\omega_2 t})|2\rangle\langle 3| + h.c.$$

$$|1'\rangle = e^{iE_1 t}|1\rangle \quad |2'\rangle = e^{i(E_1 + \omega_1 - \omega_2)t}|2\rangle \quad |3'\rangle = e^{i(E_1 + \omega_1)t}|3\rangle$$

$$H = \begin{pmatrix} 0 & 0 & \Omega_1 \\ 0 & \Delta_1 - \Delta_2 & \Omega_2 \\ \Omega_1 & \Omega_2 & \Delta_1 \end{pmatrix}$$

$$+ \begin{pmatrix} 0 & 0 & \Omega_1 e^{-2i\omega_1 t} \\ 0 & 0 & \Omega_2 e^{-2i\omega_2 t} \\ \Omega_1 e^{2i\omega_1 t} & \Omega_2 e^{2i\omega_2 t} & 0 \end{pmatrix}$$

Rotating Wave Approximation

Dressed Hamiltonian

2 photon resonance: $\delta = \Delta_1 - \Delta_2 \simeq 0$

Using

$$\tan(\theta) = \frac{\Omega_1}{\Omega_2} \quad \tan(2\phi) = \frac{\sqrt{\Omega_1^2 + \Omega_2^2}}{\Delta_1}$$

Autler Townes Splitting

$$\omega^\pm = \Delta_1 \pm \sqrt{\Delta_1^2 + \Omega_1^2 + \Omega_2^2}$$

Dressed States: $|a^+\rangle = \sin\theta \sin\phi|1\rangle + \cos\phi|3\rangle + \cos\theta \sin\phi|2\rangle$

$$|a^-\rangle = \sin\theta \cos\phi|1\rangle - \sin\phi|3\rangle + \cos\theta \cos\phi|2\rangle$$

$$|a^0\rangle = \cos\theta|1\rangle - \sin\theta|2\rangle$$

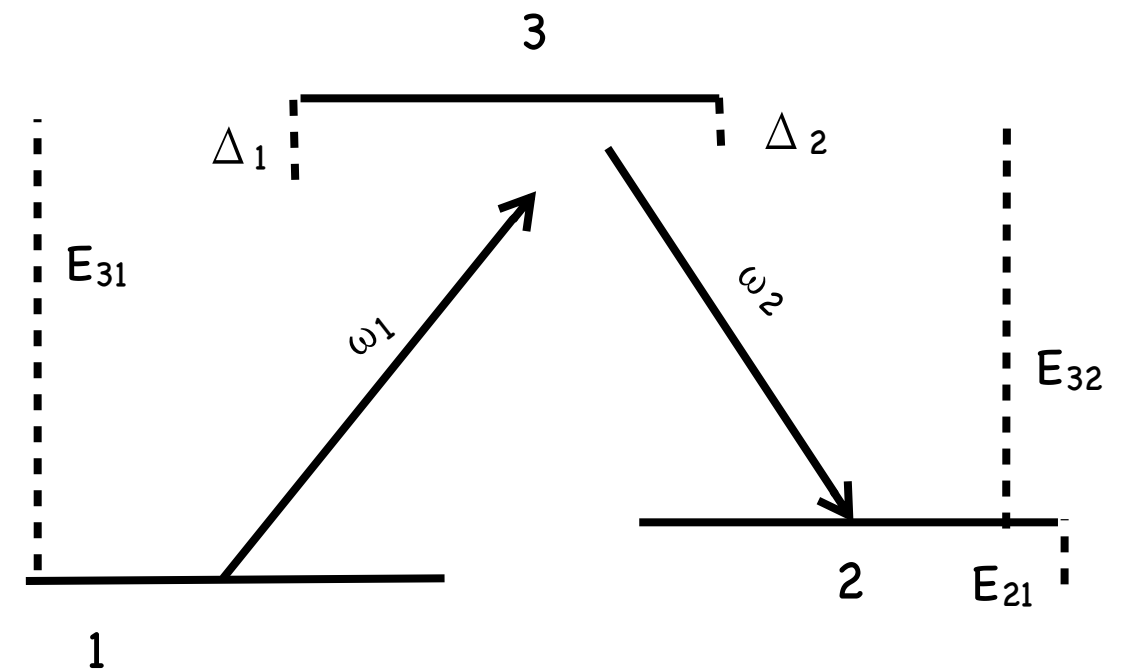
Dark State: Does not overlap with $|3\rangle$, eigenvalue 0

RWA with 3 states

$$|a^0\rangle = \cos\theta|1\rangle - \sin\theta|2\rangle$$

Dressed State

Dark State: No overlap with $|3\rangle$, eigenvalue 0

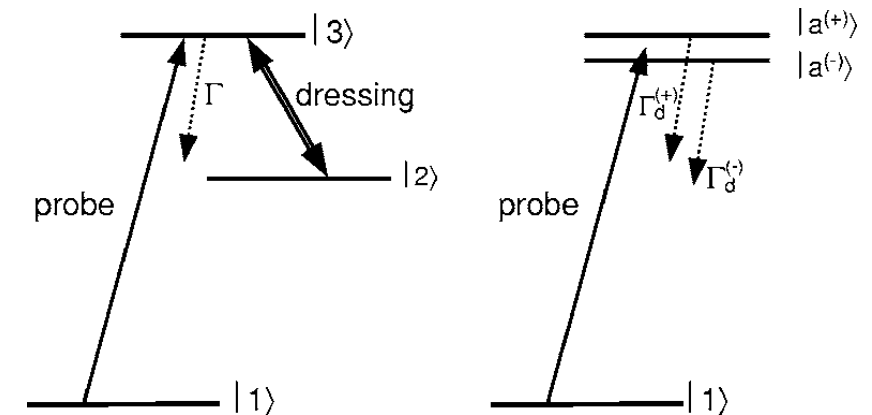


If atom is prepared in this dressed state, it cannot be excited to $|3\rangle$ and cannot decay by spontaneous emission. Hence this state is called dark state.

If by some mechanism, the atom is prepared in this state, it will remain in this state for a very long time

Consider the case : $\Omega_1 \ll \Omega_2$ $\theta \rightarrow 0$ $|a^0\rangle \rightarrow |1\rangle$

$$|a^+\rangle \rightarrow \cos\phi|3\rangle + \sin\phi|2\rangle \quad |a^-\rangle \rightarrow -\sin\phi|3\rangle + \cos\phi|2\rangle$$



Cannot excite the system even if a resonant field (between $|1\rangle$ and $|3\rangle$) is applied. This is due to the already applied dressing field between $|2\rangle$ and $|3\rangle$. This phenomenon is called Electromagnetically Induced Transparency (EIT)