Non-Adiabatic Transitions in the Density Matrix Formalism

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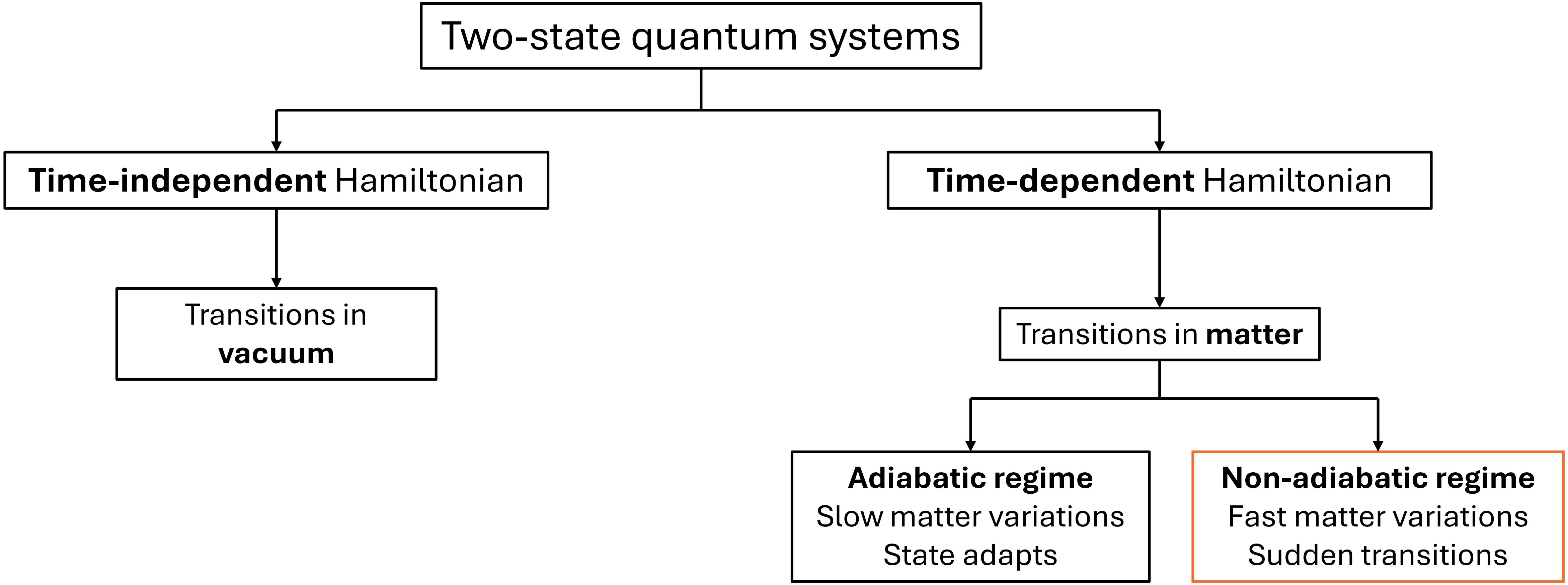
Navigating the State Transition



Goal: Derive **analytical insight** in the description of **non-adiabatic transitions** during the time-evolution of **two-state quantum systems**.

Density Matrix Formalism (Two-State Quantum System)

Schrödinger equation:
Evolves the state vector $|\psi(\mathrm{t})\rangle$

$$i\frac{\partial\psi(t)}{\partial t} = H(t)\psi(t)$$

$$\hat{\rho}(\mathrm{t}) = |\psi(\mathrm{t})\rangle\langle\psi(\mathrm{t})|$$

$\longrightarrow$

In a basis $\{|\lambda_\alpha\rangle\}_{\alpha=1,\dots,\mathrm{n}}$

von-Neumann equation:
Evolves the density matrix $\rho_{\alpha\beta}(\mathrm{t}) \equiv \langle\lambda_\alpha|\hat{\rho}(\mathrm{t})|\lambda_\beta\rangle$

$$\frac{\partial\rho(t)}{\partial t} = i\left[\rho(t), H(t)\right]$$

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Any **Hamiltonian matrix** can be written as

$$H(t) = \underbrace{\frac{E_1(t) + E_2(t)}{2} I}_{\text{Cancels in the commutator!}} + \Delta H(t)$$

Oscillation physics is in the **effective Hamiltonian**

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Parametrization in the space of Pauli matrices

$$\rho(t) = \frac{1}{2}(1+\vec{P}(t)\cdot\vec{\sigma}) \qquad \Delta H(t) = \frac{1}{2}\vec{V}(t)\cdot\vec{\sigma}$$

Basis independent!

$$\boxed{\frac{\partial\vec{P}(t)}{\partial t} = \vec{V}(t)\times\vec{P}(t)}$$

Initial Condition

$$\rho(0) = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$$

$$\Updownarrow$$

$$\vec{P}(0) = (0,0,1)$$

Bloch equation!! $\Longrightarrow$ precession of polarisation vector about potential vector.

System Hamiltonian in Interaction Basis

- **Basis Notation**

  Interaction basis : $\{|\lambda_1\rangle, |\lambda_2\rangle\}$ Energy eigenstate basis : $\{|E_1(t)\rangle, |E_2(t)\rangle\}$ *(mixing angle)*

  Basis transformation $|E_i(t)\rangle = \hat{U}(t)|\lambda_i\rangle$ with Unitary matrix, $U(t) = \begin{pmatrix} \cos\theta(t)e^{i\alpha(t)} & \sin\theta(t)e^{i[\alpha(t)+\phi(t)]} \\ -\sin\theta(t) & \cos\theta(t)e^{i\phi(t)} \end{pmatrix}$

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Specialise to **interaction basis**

$$\xrightarrow{\Delta H(t) = U(t)D_{\Delta H}(t)U^{\dagger}(t)}$$

constant $\alpha(t)$
real $\triangle$ H(t)

$$\boxed{\vec{V}(t) = \Delta E(t)(\sin 2\theta(t), 0, \cos 2\theta(t))}$$

$$\boxed{\begin{pmatrix} \dot{P}_x(t) \\ \dot{P}_y(t) \\ \dot{P}_z(t) \end{pmatrix} = \Delta E(t) \begin{pmatrix} 0 & \cos 2\theta(t) & 0 \\ -\cos 2\theta(t) & 0 & -\sin 2\theta(t) \\ 0 & \sin 2\theta(t) & 0 \end{pmatrix} \begin{pmatrix} P_x(t) \\ P_y(t) \\ P_z(t) \end{pmatrix}}$$

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In general, we can decompose Hamiltonian in time-independent & time-dependent parts:

$$\boxed{H(t) = H_0 + \mathrm{V}(t)}$$

Effective Hamiltonian:

$$\Delta H(t) = -\frac{1}{2}\Delta E_0 \begin{pmatrix} \cos 2\theta_0 - \Delta v(t) & -\sin 2\theta_0 + v_{12}(t) \\ -\sin 2\theta_0 + v_{12}^*(t) & -\cos 2\theta_0 + \Delta v(t) \end{pmatrix}$$

Recover the required form of $\vec{\mathrm{V}}(t)$ by defining the **time-dependent energy splitting** and **mixing angle**

$$\Delta E(t) = \Delta E_0 \sqrt{[\sin 2\theta_0 - v_{12}(t)]^2 + [\cos 2\theta_0 - \Delta v(t)]^2} \qquad \tan 2\theta(t) = \frac{\sin 2\theta_0 - v_{12}(t)}{\cos 2\theta_0 - \Delta v(t)}$$

[Bloch 1946]

Time-Independent Hamiltonian

The Simplest Case: $\vec{V}_0 = \Delta E_0(\sin 2\theta_0, 0, -\cos 2\theta_0)$

Trivial Solution!

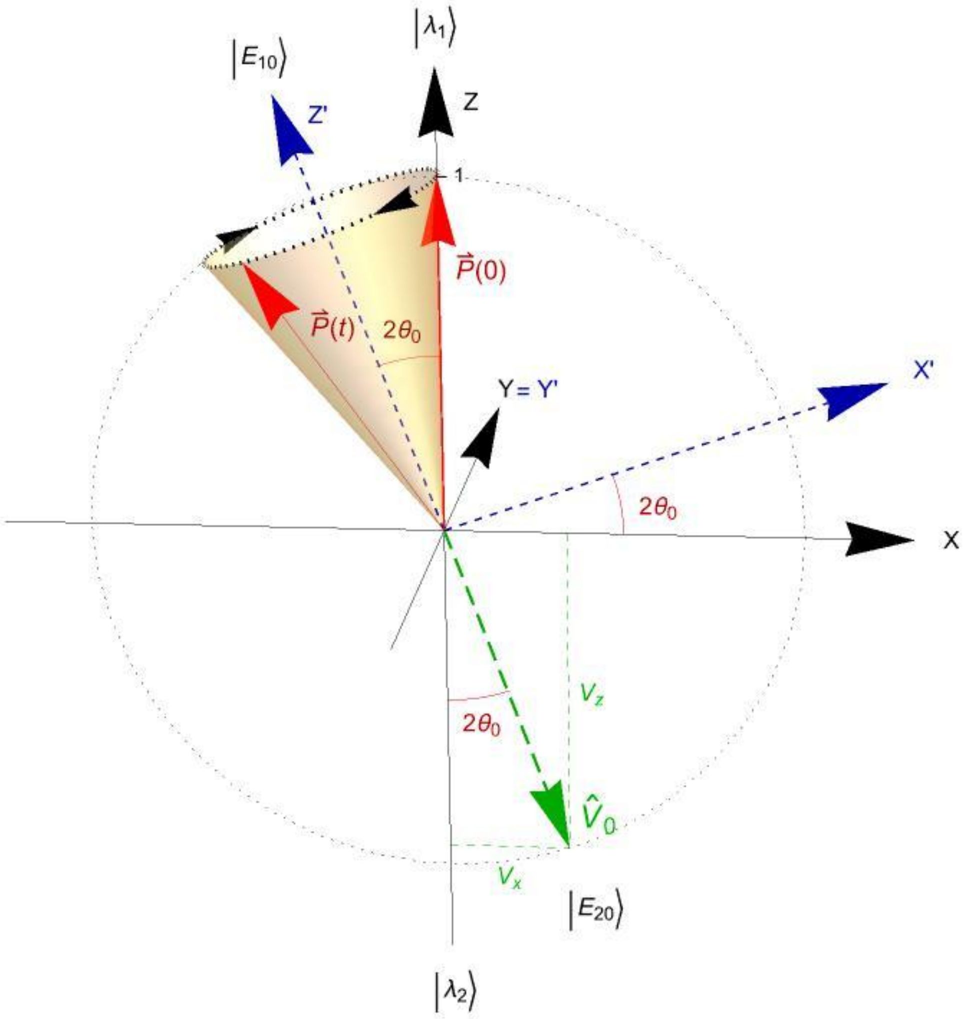
- **Probability to find the system in state $|\lambda_2\rangle$** at time t can be extracted from the z component solution by using $\rho_{22} = (1 - \mathrm{P_z})/2$

$$P_z(t) = 1 - 2\sin^2 2\theta_0 \sin^2\left(\frac{\Delta E_0 t}{2}\right)$$

$$P_{1\to 2}(t) = \rho_{22}(t) = \sin^2 2\theta_0 \sin^2\left(\frac{\Delta E_0 t}{2}\right)$$

- Application in Neutrino Physics: **Solar Neutrino Oscillations in Vacuum** where $\mathrm{l}_\odot = \mathrm{ct}$.

$$P_{\nu_e \to \nu_{\mu+\tau}} = \rho_{22} = \sin^2 2\theta_{12} \sin^2\left(\frac{\Delta m_{12}^2 l_\odot}{4E}\right)$$



Time-dependent Hamiltonian: Adiabatic Regime

- Rotating the frame $\vec{\mathrm{P}}(\mathrm{t}) \rightarrow \vec{\mathrm{P}'}(\mathrm{t}) = \mathrm{R}(\mathrm{t})\,\vec{\mathrm{P}}(\mathrm{t})$, the **modified Bloch equation** is given by

$$\begin{pmatrix} \dot{P}'_x(t) \\ \dot{P}'_y(t) \\ \dot{P}'_z(t) \end{pmatrix} = \Delta E(t) \begin{pmatrix} 0 & 1 & \frac{1}{\gamma(t)}\mathrm{sgn}(\Delta E\dot{\theta}) \\ -1 & 0 & 0 \\ \frac{1}{\gamma(t)}\mathrm{sgn}(\Delta E\dot{\theta}) & 0 & 0 \end{pmatrix} \begin{pmatrix} P'_x(t) \\ P'_y(t) \\ P'_z(t) \end{pmatrix} \Longrightarrow$$

Adiabaticity parameter

$$\gamma(t) \equiv \frac{1}{2}\left|\frac{\Delta E(t)}{\dot{\theta}(t)}\right|$$

Adiabatic regime: $\gamma \gg 1$

- **Probabilities obtained for a more general Hamiltonian** with no restrictions on diagonal and off-diagonal interactions:

$$\boxed{\begin{aligned} P_{1\to1}(t) = \rho_{11}(t) &= \frac{1}{2} + \frac{1}{2}\cos 2\theta(t)\cos 2\theta(0) + \frac{1}{2}\sin 2\theta(t)\sin 2\theta(0)\cos\left(\int_0^t \Delta E(t')dt'\right) \\ P_{1\to2}(t) = \rho_{22}(t) &= \frac{1}{2} - \frac{1}{2}\cos 2\theta(t)\cos 2\theta(0) - \frac{1}{2}\sin 2\theta(t)\sin 2\theta(0)\cos\left(\int_0^t \Delta E(t')dt'\right) \end{aligned}}$$

Application: MSW Effect in Solar Neutrinos (active-active)

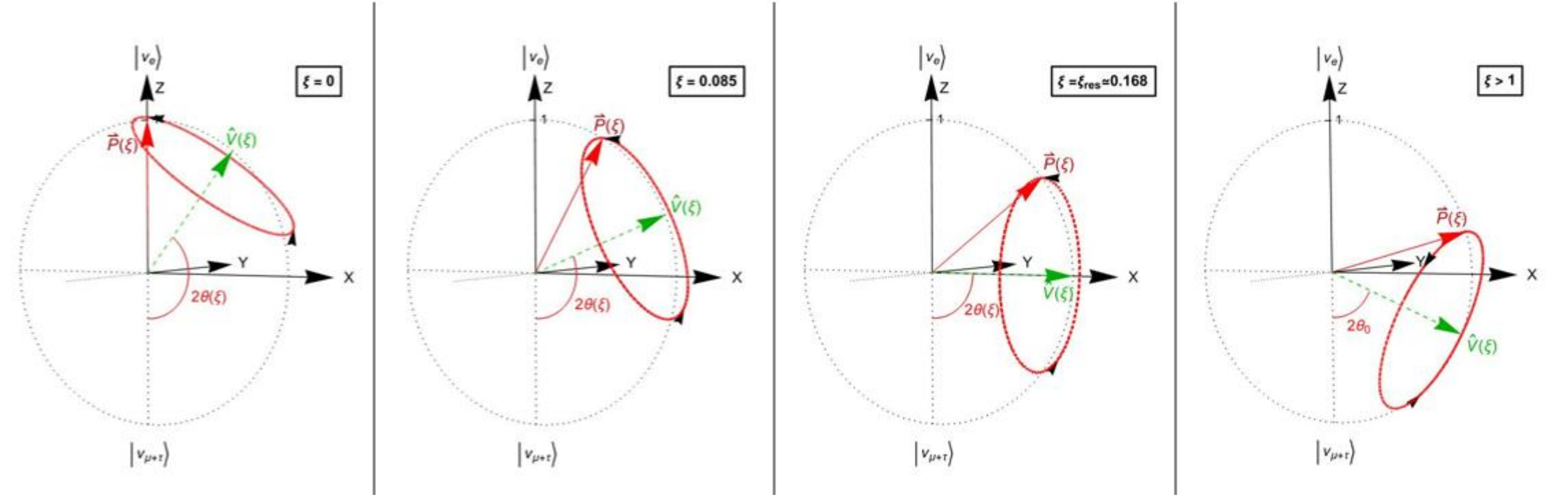
- **Time dependence** in the diagonal element, $\Delta V(t) = \sqrt{2} G_F n_e(r)$

$$P_{\nu_e \to \nu_e} = \rho_{11} \to \sin^2\theta_{12} \simeq 0.31$$
$$P_{\nu_e \to \nu_{\mu+\tau}} = \rho_{22} \to \cos^2\theta_{12} \simeq 0.69$$

Electron number density inside the Sun $\quad n_e(r) = n_e(0) e^{-8.4 \frac{r}{R_\odot}}$

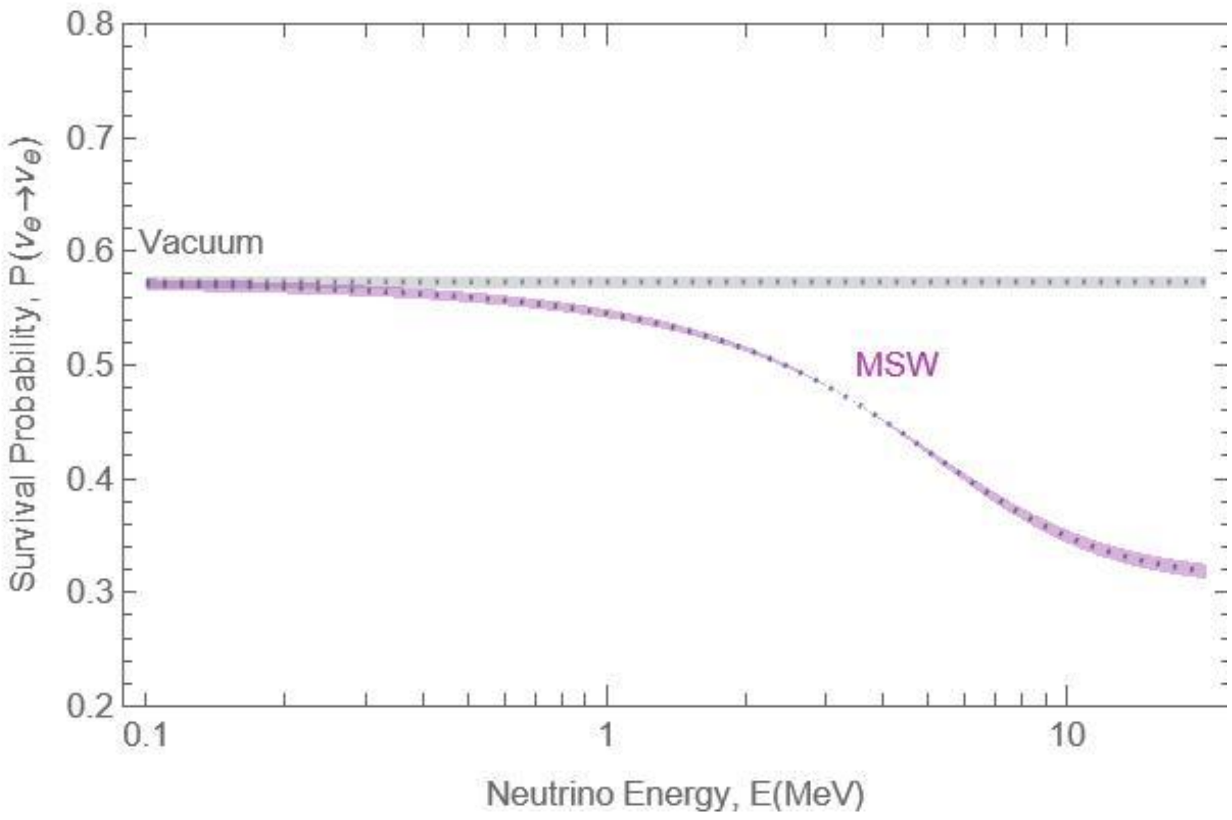
$$\xi \equiv \frac{r}{R_\odot}, \qquad \hat{V}(t) \equiv \frac{\overline{V}(t)}{\triangle E(t)}$$

Solar MSW effect with $E = 10\ MeV$



Survival Probability in Solar Neutrinos

- **Survival probability $P_{\nu_e \to \nu_e}$** of solar neutrinos as a function of the **neutrino energy E**



Low energies, Vacuum limit

High energies, MSW limit for $\theta_0 = \frac{\pi}{2}$

Time-dependent Hamiltonian

- **Retaining the $\gamma(t)$ term** in the evolution equation, the polarisation vector components are obtained by a simple change of basis:

$$P_x(t) = \int_0^t dt' \, V_x(t') P_z(t') \sin\left(\int_{t'}^t dt'' \, V_z(t'') \right)$$

$$P_y(t) = -\int_0^t dt' \, V_x(t') P_z(t') \cos\left(\int_{t'}^t dt'' \, V_z(t'') \right)$$

- In the **approximation $P_z \simeq 1$ (small mixing angle),** the crossing probability solution is

$$\boxed{\begin{aligned} P_{1\to2}(t) &= \rho_{22}(t) = \frac{1 - P_z(t)}{2} \\ &= \frac{1}{2}\int_0^t dt' \, V_x(t') \int_0^{t'} dt'' \, V_x(t'') \cos\left(\int_{t''}^{t'} dt''' \, V_z(t''') \right) \end{aligned}}$$

LZSM approximation

$$P^f_{1\to2} \simeq \frac{\pi}{2}\gamma_{res}$$

Extremely Non-Adiabatic Limit

This formula nicely interpolates between adiabatic regime, LZSM and extremely non-adiabatic limit.

Adding Interaction With Environment

Decoherence rate

- **Lindblad equation** for realistic quantum systems

$$\frac{\partial\rho(t)}{\partial t} = -i[H(t),\rho(t)] - \Gamma(t)[\sigma_z,[\sigma_z,\rho(t)]]$$

$$\frac{\partial\vec{P}(t)}{\partial t} = \vec{V}(t)\times\vec{P}(t) - \Gamma(t)[P_x\hat{x} + P_y\hat{y}]$$

- General expression for conversion probability when **including decoherence**

$$\boxed{P_{1\to 2}(t) = \rho_{22}(t) = \frac{1}{2}\int_0^t dt' V_x(t')\int_0^{t'} dt'' V_x(t'')e^{-\Gamma(t'')t''}\cos\left(\int_{t''}^{t'} dt''' V_z(t''')\right)}$$

Summary

- Derived a **general analytical expression** for **non-adiabatic two-state mixing**.
- **Unified framework**: smoothly interpolates between the Landau-Zener-Stuckelberg-Majorana (LZSM) limit with the extremely non-adiabatic limit.
- **Incorporates decoherence**, making it ready-to-use for open quantum systems.
- We plan to apply these very general results to various problems,
  1. solar active-sterile neutrino mixing,
  2. active-sterile neutrino mixing in the early universe,
  3. very heavy dark matter production from sterile-sterile neutrino mixing,
  4. photon-dark photon mixing (kinetic mixing) in the early universe……
- Density Matrix Formalism has **wider applications beyond particle physics** and serves a **general quantum mechanical description for mixing of two quantum states**.
  1. Landau-Zener transitions in Molecular/Chemical Physics,
  2. State preparation and Qubit manipulation in Quantum Information,
  3. Laser driven transitions in Atomic systems……

Thank you for listening!

Interaction Basis

- **Basis Notation**

Interaction basis : $\{|\lambda_1\rangle, |\lambda_2\rangle\}$ Energy eigenstate basis : $\{|E_1(t)\rangle, |E_2(t)\rangle\}$

Basis transformation

$$|E_i(t)\rangle = \hat{U}(t)|\lambda_i\rangle \quad \text{with Unitary matrix,} \quad U(t) = \begin{pmatrix} \cos\theta(t)e^{i\alpha(t)} & \sin\theta(t)e^{i[\alpha(t)+\phi(t)]} \\ -\sin\theta(t) & \cos\theta(t)e^{i\phi(t)} \end{pmatrix}$$

In **Neutrino Physics**, interaction basis ≡ *flavor eigenstates* and energy eigenstate basis ≡ *mass eigenstates*. U(t) corresponds to the *Leptonic mixing matrix* and θ(t) is the *mixing angle*.

Specialise to interaction basis

$$\Delta H(t) = U(t)D_{\Delta H}(t)U^{\dagger}(t) = -\frac{1}{2}\Delta E(t)\begin{pmatrix} \cos 2\theta(t) & -\sin 2\theta(t)e^{i\alpha(t)} \\ -\sin 2\theta(t)e^{-i\alpha(t)} & -\cos 2\theta(t) \end{pmatrix}$$

$$\vec{V}(t) = \Delta E(t)(\sin 2\theta(t)\cos\alpha(t), -\sin 2\theta(t)\sin\alpha(t), -\cos 2\theta(t))$$

constant α(t)
real $\triangle$ H(t)

$$\boxed{\vec{V}(t) = \Delta E(t)(\sin 2\theta(t), 0, \cos 2\theta(t))}$$

$$\boxed{\frac{\partial \vec{P}(t)}{\partial t} = \vec{V}(t) \times \vec{P}(t)}$$

$$\boxed{\begin{pmatrix} \dot{P}_x(t) \\ \dot{P}_y(t) \\ \dot{P}_z(t) \end{pmatrix} = \Delta E(t)\begin{pmatrix} 0 & \cos 2\theta(t) & 0 \\ -\cos 2\theta(t) & 0 & -\sin 2\theta(t) \\ 0 & \sin 2\theta(t) & 0 \end{pmatrix}\begin{pmatrix} P_x(t) \\ P_y(t) \\ P_z(t) \end{pmatrix}}$$

Time-dependent Mixing Angle

- How to connect this structure to the two-states systems observed in physics?

In general, we can decompose Hamiltonian in time-independent & time-dependent parts:

$$\boxed{H(t) = H_0 + \mathrm{V}(\mathrm{t})}$$

Always true!

$$\mathrm{V}(\mathrm{t}) = \begin{pmatrix} \mathrm{V}_{11}(\mathrm{t}) & \mathrm{V}_{12}(\mathrm{t}) \\ \mathrm{V}_{21}(\mathrm{t}) & \mathrm{V}_{22}(\mathrm{t}) \end{pmatrix}$$

Effective Hamiltonian:

$$\Delta H(t) = -\frac{1}{2}\Delta E_0 \begin{pmatrix} \cos 2\theta_0 - \Delta v(t) & -\sin 2\theta_0 + v_{12}(t) \\ -\sin 2\theta_0 + v_{12}^*(t) & -\cos 2\theta_0 + \Delta v(t) \end{pmatrix}$$

$$\vec{V}(t) = \Delta E_0(\sin 2\theta_0 - \mathrm{Re}[v_{12}(t)], \mathrm{Im}[v_{12}(t)], \Delta v(t) - \cos 2\theta_0)$$

Definitions

$$\triangle \mathrm{v}(\mathrm{t}) \equiv \frac{\triangle \mathrm{V}(\mathrm{t})}{\triangle \mathrm{E}_0} \qquad \mathrm{v}_{12}(t) \equiv -\frac{2\mathrm{V}_{12}(\mathrm{t})}{\triangle \mathrm{E}_0}$$

$$\triangle \mathrm{V}(\mathrm{t}) \equiv \mathrm{V}_{11}(\mathrm{t}) - \mathrm{V}_{22}(\mathrm{t})$$

$$\Delta E(t) = \Delta E_0 \sqrt{[\sin 2\theta_0 - v_{12}(t)]^2 + [\cos 2\theta_0 - \Delta v(t)]^2}$$

$$\tan 2\theta(t) = \frac{\sin 2\theta_0 - v_{12}(t)}{\cos 2\theta_0 - \Delta v(t)}$$

Recovered the structure from DMF!

$$\boxed{\vec{V}(t) = \Delta E(t)(\sin 2\theta(t), 0, \cos 2\theta(t))}$$

Ready to use!