1. Landau-Zener Problem

In this problem, our goal is to derive the expression for the probability $P_{\mathrm{LZ}} = \exp\left(-\pi \frac{h^2}{2v}\right)$ of a diabatic transition in a two-level system (i.e., finding it in its excited state) at long times, following a linear sweep.

Consider the time-dependent Hamiltonian

$$H_{\mathrm{LZ}}(t) = \frac{vt}{2}\sigma^z + \frac{h}{2}\sigma^x = \begin{pmatrix} \frac{vt}{2} & \frac{h}{2} \\ \frac{h}{2} & -\frac{vt}{2} \end{pmatrix}, \tag{1}$$

where the external Zeeman field is ramped linearly in time t at a speed v, and h sets the size of the minimum energy gap during the sweep (see sketch in lecture notes); σ^α are the Pauli matrices. The Landau-Zener(-Stueckelberg-Majorana) problem is given by the Schroedinger initial value problem

$$i\partial_t |\psi(t)\rangle = H(t)|\psi(t)\rangle, \qquad |\psi(-\infty)\rangle = |0\rangle, \qquad t \in (-\infty, +\infty). \tag{2}$$

We are interested in computing the probability of finding the two-level system in the excited state $|1\rangle$ at time $t \to +\infty$, $P_{\mathrm{LZ}} = |\langle 1|\psi(+\infty)\rangle|^2$ (so-called diabatic transition).

1.1. Use the ansatz $|\psi(t)\rangle = c_0(t)|0\rangle + c_1(t)|1\rangle$ to express P_{LZ} using the coefficients $c_{0,1}(t)$. Show that $c_1(t)$ obeys the second-order ODE

$$\ddot{c}_1(t) + \left(\frac{iv}{2} + \frac{h^2}{4} + \frac{v^2t^2}{4}\right)c_1(t) = 0. \tag{3}$$

Why is it meaningful to expand the wavefunction in the eigenstates of σ^z in the first place?

1.2. Consider the solution in the limit $t \to +\infty$; argue that the coefficient $c_1(t)$ takes the form $c_1(t) \overset{t\to\infty}{\sim} |c_1|e^{-i\varphi(t)}$ with a time-independent modulus $|c_1|$ and a time-dependent phase $\varphi(t)$. Show that, in this limit, the phase obeys the equations

$$\begin{cases} \dot{\varphi}(t) \approx \frac{vt}{2} + \frac{1}{4}\frac{h^2}{vt} + \cdots \\ \ddot{\varphi}(t) \approx \frac{v}{2} + \cdots \end{cases} \qquad \text{as} \quad t \to \pm\infty\,. \tag{4}$$

1.3. Derive the relations

$$\log\frac{c_1(+\infty)}{c_1(-\infty)} = \int_{-\infty}^{\infty} \mathrm{d}t\, \frac{\dot{c}_1(t)}{c_1(t)}, \qquad \frac{\dot{c}_1(t)}{c_1(t)} \overset{|t|\to\infty}{\sim} -i\left(\frac{vt}{2} + \frac{1}{4}\frac{h^2}{vt}\right), \tag{5}$$

and use the left-hand-side equality to express the LZ probability P_{LZ}.

1.4. To compute the integral by only knowing the ratio $\dot{c}_1(t)/c_1(t)$ in the limit $|t| \to \infty$, we will use contour integration. To this end, apply analytic continuation $t \mapsto z \in \mathbb{C}$, and go polar using the parametrization $z = Re^{i\theta}$. Then use the residue theorem (see Fig. 1) to show that

$$\log\frac{c_1(+\infty)}{c_1(-\infty)} = -\pi\frac{h^2}{4v}\,. \tag{6}$$

Last, derive the expression for P_{LZ}.

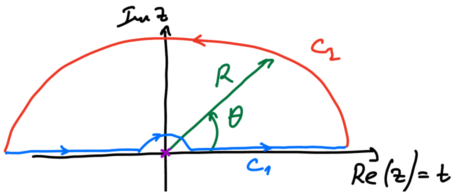

Figure 1: Analytic continuation in the complex plane $\mathbb{C}$, with two contours C_1 and C_2.

2. Adiabatic Gauge Potentials for a general 2LS

In this problem, we will formally derive the expression for the adiabatic gauge potential using calculus. Consider the general 2LS Hamiltonian $H_{\rm ctrl}(\theta,\varphi) = E\hat{n}(\theta,\varphi)\cdot\vec{\sigma}$ where the unit vector $\hat{n}(\theta,\varphi)$ is parametrized in spherical coordinates (θ,φ), $\vec{\sigma}$ is the vector of Pauli matrices, and $\pm E$ are the eigenenergies. You can think of $(\theta(t),\varphi(t))$ as parameters that we can change in time according to some arbitrary protocol.

2.1. Derive the expression for the intantaneous eigenstates

$$H_{\rm ctrl}(\theta,\varphi)\,|\psi_\pm[\theta,\varphi]\rangle = \pm E\,|\psi_\pm[\theta,\varphi]\rangle\,.$$

Construct the unitary transformation $U(\theta,\varphi)$ that diagonalizes the instantaneous Hamiltonian $H_{\rm ctrl}(\theta,\varphi)$.

2.2. Now, recall that the parameters $(\theta(t),\varphi(t))$ change in time according to some arbitrary schedule. Write down the Hamiltonian $\tilde{H}_{\rm ctrl}(\theta,\varphi)$ in the co-moving frame and identify the moving-frame gauge potentials $\tilde{\mathcal{A}}_\theta(\theta,\varphi), \tilde{\mathcal{A}}_\varphi(\theta,\varphi)$.

2.3. Evaluate algebraically the moving-frame gauge potentials $\tilde{\mathcal{A}}_\theta(\theta,\varphi), \tilde{\mathcal{A}}_\varphi(\theta,\varphi)$; then go back to the lab frame and find the lab-frame gauge potentials $\mathcal{A}_\theta, \mathcal{A}_\varphi$. Verify that they act on the instantaneous eigenstates as a derivative, e.g., $\mathcal{A}_\varphi\,|\psi_\pm[\theta,\varphi]\rangle = i\partial_\varphi\,|\psi_\pm[\theta,\varphi]\rangle$.

2.4. Compute the Kato gauge potentials $\mathcal{A}_{K,\theta}, \mathcal{A}_{K,\varphi}$. Explain in which sense the Kato gauge potential corresponds to a covariant derivative (think of the analogy with electromagnetism).

2.5. Write down the counter-diabatic Hamiltonians for the gauge potentials $\mathcal{A}, \mathcal{A}_K$; why is the CD Hamiltonian not unique? What does this imply physically?

2.6. Apply a re-phasing $U(1)$ gauge transformation on the individual eigenstates,

$$|\psi_\pm[\theta,\varphi]\rangle \mapsto e^{i\chi_\pm(\theta,\varphi)}\,|\psi_\pm[\theta,\varphi]\rangle\,. \tag{7}$$

Show explicitly that the gauge potentials $\mathcal{A}_\theta, \mathcal{A}_\varphi$ change, while their Kato counterparts $\mathcal{A}_{K,\theta}, \mathcal{A}_{K,\varphi}$ are gauge-invariant under this transformation.

2.7. *"What I cannot create, I do not understand"*, Richard P. Feynman.

Write your own code to explicitly verify numerically the accumulated phases from Table 1 below for the two-level system; use the periodic trajectory

$$\hat{n}(\theta_*,\varphi(t)) = (\sin\theta_*\cos\omega t,\ \sin\theta_*\sin\omega t,\ \cos\theta_*)^t$$

for a time-independent $\theta_* = \pi/3$ and $\varphi(t) = \omega t$, with $t\in[0,T]$ $(T = 2\pi/\omega)$. The definitions of the dynamical and geometric phases in Table 1 are

$$\begin{aligned}\phi_\pm(t) &= \int_0^t E_\pm(\lambda(s))\,\mathrm{d}s\,,\\ \gamma_\pm(t) &= \int_{\lambda(0)}^{\lambda(t)} \langle\psi_\pm[\lambda]|i\partial_\lambda\psi_\pm[\lambda]\rangle\,\mathrm{d}\lambda\,.\end{aligned} \tag{8}$$

Which Hamiltonian $\mathcal{H}$ do we have to evolve with, if the wavefunction is supposed to accumulate no phase after one period T at all?

drive	*Hamiltonian $\mathcal{H}(t)$*	*accumulated phase*
adiabatic $T_{\mathrm{ramp}}{\to}\infty$	H_{ctrl}	$\gamma_n(t)+\phi_n(t)$
dyn. counterdiabatic $\chi_n(t){=}0$	$H_{\mathrm{ctrl}}+\mathcal{A}_\lambda$	$\phi_n(t)$
Kato counterdiabatic gauge-invariant	$H_{\mathrm{ctrl}}+\mathcal{A}_{K,\lambda}$	$\gamma_n(t)+\phi_n(t)$
generic counterdiabatic χ_n arbitrary	$H_{\mathrm{ctrl}}+\mathcal{A}'_\lambda$	$\chi_n(t){+}\phi_n(t)$
Kato AGP gauge-invariant	$\mathcal{A}_{K,\lambda}$	$\gamma_n(t)$
periodic AGP $\chi_n(t){=}2\pi\ell_n t/T$	$\mathcal{A}(t){=}\mathcal{A}(t{+}T)$	$2\pi\ell_n$, $\ell_n{\in}\mathbb{Z}$ (at $t{=}T$)

Table 1: Adiabatic gauges. Summary of common gauge choices (first column) and the resulting accumulated phases (third column) for the Schroedinger equation $i\partial_t\,|\psi_n(t)\rangle{=}\mathcal{H}(\lambda(t))\,|\psi_n(t)\rangle$, with $\mathcal{H}(t)$ given in the second column above. Independent of the gauge choice for the *adiabatic gauge potential* (AGP) $\mathcal{A}$, the AGP induces transitionless driving between eigenstates of H_{ctrl}; however, the gauge choice determines the accumulated phase. The dynamical phase is $\phi_n(t)$, the geometric phase is $\gamma_n(t)$, and $\chi_n(\lambda(t))$ is an arbitrary smooth function; the periodic gauge is only well-defined for periodic control with $\ell_n{\in}\mathbb{Z}$. Here $\lambda(t)=\varphi(t)$ with $\theta=\theta_*$ is kept fixed (see problem 2.7 above), and the gauge potential $\mathcal{A}'_\lambda$ is obtained from $\mathcal{A}=(i\partial_\lambda U_\lambda)U_\lambda^\dagger$ by applying the re-phasing gauge transformation specified in the left column, see also Eq. (7); i.e., we measure χ_n w.r.t. the phase accumulated by $\mathcal{A}$.