# CHEM2504 HW 2

**Due: Mar 19, 3:00 pm, 2024**

Following previous Homework of the TLS (two-level system) with the perturbed Hamiltonian $H(t) = \begin{bmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{bmatrix}$, where the off-diagonal term $\gamma e^{i\omega t}$ is in the same role of $V$ in HW1. Numerically and analytically, the wavefunction with such Hamiltonian can also be solved exactly.

The time-dependent wavefunction can be expanded as $|\psi(t)\rangle = C_1(t)\,|\phi_1\rangle + C_2(t)\,|\phi_2\rangle$ where $\phi_i$ is the basis function. $C_1(t=0) = 1$ and $C_2(t=0) = 0$ ; $|\psi(t)\rangle$ follows Schrödinger's equation

1. Show that the evolution of $|\psi(t)\rangle$ can be written in the following form:

$$\begin{bmatrix} \dot{C}_1(t) \\ \dot{C}_2(t) \end{bmatrix} = -\frac{i}{\hbar} \begin{bmatrix} H_{11}(t) H_{12}(t) \\ H_{21}(t) H_{22}(t) \end{bmatrix} \begin{bmatrix} C_1(t) \\ C_2(t) \end{bmatrix} \tag{1}$$

   where $H_{ij}(t) = \langle\phi_i|\, H(t)\, |\phi_j\rangle$.

2. Assuming when $t = 0$, $C_1(t=0) = 1$, $C_2(t=0) = 0$, $\hbar\omega = 0.12$ eV, $\gamma = 0.02$ eV, $E_1 = -0.1$ eV, $E_2 = 0.1$ eV. Using the numerical method to evolve the wavefunction and solve equ.1 (You can solve equ.1 by using up to 3rd-order of $\dot{C}(t)$ expansions. Choose an appropriate $dt$ when doing the evolution.) Plot $|C_1(t)|^2$ and $|C_2(t)|^2$ as a function of time.

3. Compare the above plots with the exact formula (Rabi oscillation formula from last week).