CHEM2504 HW 4

Due: Apr. 2, 3:00 pm, 2024

For the time-dependent TLS (two level system) with the Hamiltonian $H(t) = \begin{bmatrix} E_1 & \gamma e^{i\omega t - \eta t} \\ \gamma e^{-i\omega t - \eta t} & E_2 \end{bmatrix}$, $E_1 < E_2$ and γ is a real number.

Set $E_1 = -0.1$ eV, $E_2 = 0.1$ eV, $\gamma = 0.02$ eV, and $\eta = 0.001$ fs^{-1}. Now the perturbation has the decaying term $-\eta t$. Starting the wavefunction from $|\psi(t=0)\rangle = |\phi_1\rangle$ (i.e. $C_1(t=0) = 1$), compute the following quantities:

1. Using the evolution method by solving the Schrödinger's equation (e.g. method in HW3), at different $\hbar\omega$ (for example, you can sample $\hbar\omega$= 0.01, 0.03, 0.05, ..., 0.41 eV), solve the final $|C_2(t=\infty)|^2$ occupation. (You may want to run the calculation long enough so that the perturbation is already too small to make a difference to the occupations. Check the time-evolving occupation to decide the appropriate stopping time.)

2. Plot the final results of $|C_2(t=\infty)|^2$ as a function of oscillating energy (i.e. $\hbar\omega$), and fit such curve using a Lorentzian distribution ($y = \Gamma/(x^2 + \Gamma^2)$). What is the relation between η and Γ.