CHEM2504 HW 3

Due: Mar 26, 3:00 pm, 2024

For the time-dependent TLS (two level system) with the Hamiltonian $H(t) = \begin{bmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{bmatrix}$, $E_1 < E_2$ and γ is a real number. Let's try to evolve the wavefunction following the expansion of the time-evolution operator U up to 2 ps. Set $E_1 = -0.1$ eV, $E_2 = 0.1$ eV, $\gamma = 0.02$ eV , $\hbar\omega = 0.12$ eV. Write the wavefunction as $|\psi(t)\rangle = C_1(t)\,|\phi_1\rangle + C_2(t)\,|\phi_2\rangle$ and start from $|\psi(t=0)\rangle = |\phi_1\rangle$ (i.e. $C_1(t=0) = 1$).

1. Expand U to the 1st-order. For every time-step, compute $|C_1(t)|^2$, $|C_2(t)|^2$, and $|C_1(t)|^2 + |C_1(t)|^2$ with $\Delta t = 1$ fs, $\Delta t = 0.1$ fs, and $\Delta t = 0.01$ fs, respectively.

2. Now using up to the 2nd-order expansion of U, repeat the above calculations and plots, what is the appropriate dt used to yield reasonable results (e.g. the normalization of the wavefunction is very close to 1 along the whole evolution process)?

3. Compare the above best results with the exact results (either from last homework or from analytical formula).