

CHEM2504 HW 8

Due: May 28, 3:00 pm, 2024

Use the parameters from HW5 (Set $E_1 = -0.1$ eV, $E_2 = 0.1$ eV, $\gamma = 0.02$ eV, $\hbar\omega = 0.12$ eV and $\eta = 0.001$ fs⁻¹), solve the density matrix evolution exactly using the numerical method. Here, the off-diagonal elements suffer from the decoherence characterized by the decoherence time τ . Plot the occupation of state 2 (ρ_{22}) after a long time (assuming the initial occupation is on state 1) under different excitations. For example, $\hbar\omega$ can take the values from 0.06 eV to 0.34 eV every 0.02 eV and the plot has x-axis of $\hbar\omega$ and y-axis of $\rho_{22}(t \rightarrow \infty)$. Plot such graph for the following decoherence time $\tau = 5, 15, 25, 50, 100, 500$ fs. What is your observation for the trend of the occupation line shape (i.e. occupations excited by different frequencies) with the increasing decoherence time?