Chem. 550
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BASICS – COMPUTER ASSIGNMENT 1

Consider a two-level system (TLS) whose Hamiltonian in the site representation is given by

$$H = -\hbar\Omega\left(|R\rangle\langle L| + |L\rangle\langle R|\right) + \varepsilon\left(|R\rangle\langle R| - |L\rangle\langle L|\right)$$

where $|R\rangle, |L\rangle$ are right- and left-localized states and $\Omega, \varepsilon > 0$. Write the matrix of the Hamiltonian. Set $\hbar = 1$ and use a symbolic algebra problem to perform the following operations:

(a) Diagonalize the 2×2 Hamiltonian matrix to obtain the eigenvectors (which give the eigenstates $|\Phi_0\rangle, |\Phi_1\rangle$) and eigenvalues E_0, E_1. Check that the results revert to those from BASICS PROBLEM 3 in the special case $\varepsilon = 0$.

(b) Suppose the TLS is initially in the right-localized state $|\Psi(0)\rangle = |R\rangle$. Express this state in terms of the two eigenstates and compute $|\Psi(t)\rangle$. Also calculate and plot the probability to find the system in the right-localized state as time progresses. For $\varepsilon = 0$ check against your analytical results from BASICS PROBLEM 3. Comment on any differences in the behavior you observe. Roughly at what magnitude of ε (compared to $\hbar\Omega$) do you begin to observe qualitatively different eigenstates and dynamics compared to the case of a symmetric TLS ($\varepsilon = 0$)?

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