Chem. 550
Instructor: Nancy Makri

BASICS PROBLEM 3

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

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

where $|R\rangle, |L\rangle$ are right- and left-localized states and $\Omega > 0$.

(a) Construct and diagonalize the 2×2 Hamiltonian matrix to obtain the eigenstates $|\Phi_0\rangle, |\Phi_1\rangle$ with eigenvalues E_0, E_1 (ordered such that $E_0 < E_1$).

For the remaining of this problem, assume that the TLS is prepared in the right-localized state $|R\rangle$. We want to propagate this state, i.e. find $|\Psi(t)\rangle$, and to calculate the probability amplitudes of finding the system in the right-localized state and in the left-localized state as a function of time. We will approach this in three different ways:

(b) By expressing the initial state as a linear combination of eigenstates and propagating each of the eigenstates individually. Write

$$|\Psi(t)\rangle = c_0(t)|\Phi_0\rangle + c_1(t)|\Phi_1\rangle,$$

identify the coefficients, and calculate the amplitudes $\langle R|\Psi(t)\rangle$ and $\langle L|\Psi(t)\rangle$.

(c) By working in the $|R\rangle, |L\rangle$ basis. The expansion of the wavefunction is

$$|\Psi(t)\rangle = c_R(t)|R\rangle + c_L(t)|L\rangle.$$

Write down the coupled differential equations for the two expansion coefficients. The system of differential equations can be solved easily by differentiating one more time. This way the equations decouple. From the differential equation for each coefficient write the general solution and apply boundary conditions. (Hint: this is a second order differential equation, so you need to apply two boundary conditions, for the expansion coefficient and its derivative.) Confirm that the result of this treatment agrees with the results from part (b).

(d) Use the spectral expansion to obtain the time evolution operator. Calculate the matrix elements of the time evolution operator (i.e., the propagator) in the left/right representation. Show explicitly that the resulting propagator matrix is unitary.

(e) Show that the propagated state in the left/right representation obtained in part (c) satisfies the time-dependent Schrödinger equation.

(f) Find the survival probability as a function of time.