Chem. 542
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Computer Assignment 1

Evolution using basis sets

Consider the rotation of a methyl group, which is described by a potential with three identical wells and cyclic boundary conditions. We will treat this within a three-state approximation. The three degenerate, localized states, which we call $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ have energies equal to zero, and each of them is coupled to its nearest neighbors via matrix elements which we set equal to -1 in some units. Use Mathematica or other symbolic algebra software to perform the following calculations.

(a) Calculate the eigenstates $|\Psi_1\rangle, |\Psi_2\rangle, |\Psi_3\rangle$ and eigenvalues of this system.

(b) Express $|\phi_1\rangle$ in terms of the eigenstates of the Hamiltonian. Using this form, calculate the time evolution of this initial state and calculate its survival amplitude and the survival probability. Plot your result.