

Chem. 540
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PROBLEM FORMALISM 15

Consider a two-state system described by the Hamiltonian \hat{H} which is given by the expression (in eV)

$$\hat{H} = -(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|)$$

where ϕ_1, ϕ_2 are orthonormal basis states.

- Find the eigenvalues of this Hamiltonian.
- Find the eigenstates.
- Write the spectral expansion of the Hamiltonian.
- Construct the matrix of eigenvectors. Show explicitly that this matrix is unitary.

Reminder:

The spectral expansion of an operator is its expression in terms of its own eigenstates and eigenvalues. This is derived by putting the resolution of identity (in terms of eigenstates) next to the operator, i.e. if

$$\hat{H}|\Phi_n\rangle = E_n|\Phi_n\rangle$$

Then the spectral expansion is

$$\hat{H} = \hat{H} \sum_n |\Phi_n\rangle\langle\Phi_n| = \sum_n E_n |\Phi_n\rangle\langle\Phi_n|.$$