F2011

PROBLEM 6: Variational Method

Consider a Hamiltonian H that may or may not be solved exactly. The variational theorem states that the expectation value of energy obtained from a trial wavefunction will always be greater than or equal to the ground state energy.

Consider a trial wave function ϕ consisting of two basis wavefunctions Ψ_1 and Ψ_2 such that

$$\phi = c_1\Psi_1 + c_2\Psi_2$$

where c_1 and c_2 are constants.

(a) Find the expectation value of the energy for this system. [1 point]

(b) Now assume $\langle\Psi_1|\Psi_2\rangle = \langle\Psi_2|\Psi_1\rangle = 0$, $\langle\Psi_1|H|\Psi_2\rangle = \langle\Psi_2|H|\Psi_1\rangle$ and c_1 and c_2 are real. Determine a 2x2 matrix relationship for the best bound on the energy. [3 points]

(c) Now also assume Ψ_1 and Ψ_2 are orthonormal. Solve the matrix relationship you found in part (b) to determine 2 solutions for the best bound energy. [2 points]

(d) Note that there are 2 solutions to the best bound energy found in part (c). What additional constraint can you apply to remove one of the solutions? [2 points]

(e) Confirm your answer to part (c) by using a Simple Harmonic Oscillator Hamiltonian and setting Ψ_1 to be the ground state eigenfunction and Ψ_2 to be the first excited state eigenfunction of the Simple Harmonic Oscillator [2 points]

(a)

We let

$$|\phi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle,$$

where c_1 and c_2 are constants. We want to determine

$$\langle H\rangle = \langle\phi|H|\phi\rangle.$$

So

$$\langle\phi|H|\phi\rangle = \left(c_1^*\langle\psi_1| + c_2^*\langle\psi_2|\right)H\left(c_1|\psi_1\rangle + c_2|\psi_2\rangle\right)$$

$$= |c_1|^2\langle\psi_1|H|\psi_1\rangle + |c_2|^2\langle\psi_2|H|\psi_2\rangle + c_1^*c_2\langle\psi_1|H|\psi_2\rangle + c_2^*c_1\langle\psi_2|H|\psi_1\rangle$$

Let

$$H|\psi_1\rangle = E_1|\psi_1\rangle$$

and

$$H|\psi_2\rangle = E_2|\psi_2\rangle.$$

Then

$$\langle\phi|H|\phi\rangle = |c_1|^2\langle\psi_1|E_1|\psi_1\rangle + |c_2|^2\langle\psi_2|E_2|\psi_2\rangle + c_1^*c_2\langle\psi_1|E_2|\psi_2\rangle + c_2^*c_1\langle\psi_2|E_1|\psi_1\rangle$$

$$= |c_1|^2E_1\langle\psi_1|\psi_1\rangle + |c_2|^2E_2\langle\psi_2|\psi_2\rangle + c_1^*c_2E_2\langle\psi_1|\psi_2\rangle + c_2^*c_1E_1\langle\psi_2|\psi_1\rangle$$

$$\boxed{\langle\phi|H|\phi\rangle = |c_1|^2E_1 + |c_2|^2E_2}.$$

(I assumed $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthonormal because the problem explicitly says they're basis wavefunctions, which implies orthonormality.)