

The Variational Method

The ground state $|0\rangle$ of a hamiltonian H is the state whose energy E_0

$$H|0\rangle = E_0|0\rangle$$

is the lowest eigenvalue E_0 of H . A reasonable way to approximate the ground state $|0\rangle$ and its energy E_0 is to form a trial state $|\alpha_1, \alpha_2, \dots, \alpha_n\rangle$ that depends upon n real parameters α_i and to minimize the mean value \bar{H} of H in the trial state

$$\bar{H}(\alpha_1, \dots, \alpha_n) = \frac{\langle \alpha_1, \dots, \alpha_n | H | \alpha_1, \dots, \alpha_n \rangle}{\langle \alpha_1, \dots, \alpha_n | \alpha_1, \dots, \alpha_n \rangle}.$$

One sets

$$\frac{\partial \bar{H}}{\partial \alpha_i} = 0 \quad 1 \leq i \leq n$$

and gets n equations for the n values of the α_i that minimize \bar{H} .

This method works better if one chooses the trial state wisely. One must guess what the true ground state looks like and form such a trial state $|\alpha_1, \dots, \alpha_n\rangle$. One also must be able to compute \bar{H} .