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 $|\alpha_1, \alpha_2, \ldots, \alpha_n\rangle$ that depends upon $n > 1$ parameters $\alpha_i$ and to minimize the mean value $\bar{H}$ of $H$ in the trial state

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

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 $\alpha_i$ 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 $|\alpha_1, \ldots, \alpha_n\rangle$. One also must be able to compute $\bar{H}$. 