The Variational Method

The variational method is a robust way of finding the ground state—at least in a system of a finite number of degrees of freedom—and also the next excited state, and then the one after that.

The ground state $|0\rangle$ is the state in which the hamiltonian H assumes its least e-val E_0, and so it minimizes the ratio

$$\frac{\langle 0|H|0\rangle}{\langle 0|0\rangle} = E_0. \tag{1}$$

Thus any approximation $|a_1, a_2, \ldots\rangle$ to the ground state $|0\rangle$ that may depend upon one or more parameters $a_1, a_2, \ldots$ will have a higher mean value of H than that E_0 of the ground state $|0\rangle$

$$\langle a_1, a_2, \ldots |H| a_1, a_2, \ldots\rangle / \langle a_1, a_2, \ldots | a_1, a_2, \ldots\rangle \geq E_0. \tag{2}$$

The key to using the variational method is to pick a sensible trial ground state $|a_1, a_2, \ldots\rangle$ depending upon one or more parameters. The best values of the parameters are those that minimize the ratio (2), that is, those for which the derivatives

$$\frac{\partial \left(\langle a_1, a_2, \ldots |H| a_1, a_2, \ldots\rangle / \langle a_1, a_2, \ldots | a_1, a_2, \ldots\rangle\right)}{\partial a_i} = 0 \tag{3}$$

all vanish.

Once one has found a suitable approximate ground state $|a_1, a_2, \ldots\rangle$, one may again use the variational method to find an approximate first-excited state $|b_1, b_2, \ldots\rangle$. It will be the one that is orthogonal to the approximate ground state $|a_1, a_2, \ldots\rangle$ and that minimizes the ratio

$$\langle b_1, b_2, \ldots |H| b_1, b_2, \ldots\rangle / \langle b_1, b_2, \ldots | b_1, b_2, \ldots\rangle \geq E_1. \tag{4}$$

Next one may look for states of least energy that are orthogonal to both $|a_1, a_2, \ldots\rangle$ and $|b_1, b_2, \ldots\rangle$.

The variational method, when done fully, leads to the stationary-state Heisenberg equation. To see how, let's consider an arbitrary variation $\delta|\psi\rangle$ to our sought-after ground state $|\psi\rangle$. If we've actually got the real ground state, then the variation of the ratio (1)

$$\delta\left(\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right) = 0 \tag{5}$$

would vanish for all variations $|\delta\psi\rangle$ of the trial state. That is,

$$\frac{\langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle\left(\langle\delta\psi|\psi\rangle + \langle\psi|\delta\psi\rangle\right)}{\langle\psi|\psi\rangle^2} = 0 \tag{6}$$

or

$$\langle\delta\psi|H|\psi\rangle + \langle\psi|H|\delta\psi\rangle - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\left(\langle\delta\psi|\psi\rangle + \langle\psi|\delta\psi\rangle\right) = 0. \tag{7}$$

Replacing $|\delta\psi\rangle$ by $i|\delta\psi\rangle$, we find

$$-i\langle\delta\psi|H|\psi\rangle + i\langle\psi|H|\delta\psi\rangle - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\left(-i\langle\delta\psi|\psi\rangle + i\langle\psi|\delta\psi\rangle\right) = 0. \tag{8}$$

Half the sum of (7) and $i\times$(8) is

$$\langle\delta\psi|H|\psi\rangle - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\langle\delta\psi|\psi\rangle = 0. \tag{9}$$

Since this equation must hold for all variations $\langle\delta\psi|$, we may elevate it to the vector equation

$$H|\psi\rangle - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle = 0 \tag{10}$$

which we recognize as the stationary-state Heisenberg equation with e-val

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{11}$$