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 eigenvalue $E_0$, and so it minimizes the ratio

$$\frac{\langle 0|H|0 \rangle}{\langle 0|0 \rangle} = E_0.$$  \hspace{1cm} (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 $|0\rangle$

$$\langle a_1, a_2, \ldots |H|a_1, a_2, \ldots \rangle / \langle a_1, a_2, \ldots |a_1, a_2, \ldots \rangle \geq E_0.$$  \hspace{1cm} (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

$$\frac{\partial \left( \frac{\langle a_1, a_2, \ldots |H|a_1, a_2, \ldots \rangle}{\langle a_1, a_2, \ldots |a_1, a_2, \ldots \rangle} \right)}{\partial a_i} = 0$$  \hspace{1cm} (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

$$\langle b_1, b_2, \ldots |H|b_1, b_2, \ldots \rangle / \langle b_1, b_2, \ldots |b_1, b_2, \ldots \rangle \geq E_1.$$  \hspace{1cm} (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 $\delta \psi$ to our sought-after ground state $|\psi\rangle$. If we’ve actually got the real ground state, then the variation of the ratio (1)

$$\delta \left( \frac{\langle \psi|H|\psi \rangle}{\langle \psi|\psi \rangle} \right) = 0$$  \hspace{1cm} (5)
would vanish for all variations $|\delta \psi\rangle$ of the trial state. That is,
\[
\frac{\langle \delta \psi | H | \psi \rangle + \langle \psi | H | \delta \psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \psi | H | \psi \rangle (\langle \delta \psi | \psi \rangle + \langle \psi | \delta \psi \rangle)}{\langle \psi | \psi \rangle^2} = 0
\]
(6)
or
\[
\langle \delta \psi | H | \psi \rangle + \langle \psi | H | \delta \psi \rangle - \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} (\langle \delta \psi | \psi \rangle + \langle \psi | \delta \psi \rangle) = 0.
\]
(7)
Replacing $|\delta \psi\rangle$ by $i|\delta \psi\rangle$, we find
\[
-i \langle \delta \psi | H | \psi \rangle + i \langle \psi | H | \delta \psi \rangle - \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} (-i \langle \delta \psi | \psi \rangle + i \langle \psi | \delta \psi \rangle) = 0.
\]
(8)
Half the sum of (7) and $i \times$ (8) is
\[
\langle \delta \psi | H | \psi \rangle - \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \langle \delta \psi | \psi \rangle = 0.
\]
(9)
Since this equation must hold for all variations $\langle \delta \psi |$, we may elevate it to the vector equation
\[
H | \psi \rangle - \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} | \psi \rangle = 0
\]
(10)
which we recognize as the stationary-state Heisenberg equation with e-val
\[
E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}.
\]
(11)