The Variation Theorem in Dirac Notation

The recipe for calculating the expectation value for energy using a trial wave function is,

$$\langle E \rangle = \langle \Psi | \hat{H} | \Psi \rangle \tag{1}$$

Now suppose the eigenfunctions of $\hat{H}$ are denoted by $|i\rangle$. Then,

$$\hat{H} |i\rangle = \varepsilon_i |i\rangle = |i\rangle \varepsilon_i \tag{2}$$

Next we write $|\Psi\rangle$ as a superposition of the eigenfunctions $|i\rangle$,

$$|\Psi\rangle = \sum_i |i\rangle\langle i|\Psi\rangle \tag{3}$$

and substitute it into equation (1).

$$\langle E \rangle = \sum_i \langle \Psi | \hat{H} | i\rangle\langle i|\Psi\rangle \tag{4}$$

Making use of equation (2) yields,

$$\langle E \rangle = \sum_i \langle \Psi | i\rangle \varepsilon_i \langle i|\Psi\rangle \tag{5}$$

After rearrangement we have,

$$\langle E \rangle = \sum_i \varepsilon_i \left|\langle i|\Psi\rangle\right|^2 \tag{6}$$

However, $\left|\langle i|\Psi\rangle\right|^2$ is the probability that ε_i will be observed, p_i.

$$\langle E \rangle = \sum_i \varepsilon_i p_i \geq \varepsilon_0 \tag{7}$$

Thus, the expectation value obtained using the trial wave function is an upper bound to the true energy. In other words, in valid quantum mechanical calculations you can’t get a lower energy than the true energy.