

10.3: The Variation Theorem in Dirac Notation

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

$$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle \quad (10.3.1)$$

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

$$\hat{H}|i\rangle = \varepsilon_i |i\rangle = |i\rangle \varepsilon_i \quad (10.3.2)$$

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

$$|\psi\rangle = \sum_i |i\rangle \langle i | \psi \rangle$$

and substitute it into Equation 10.3.1.

$$\langle E \rangle = \sum_i \langle \psi | \hat{H} | i \rangle \langle i | \psi \rangle$$

Making use of Equation 10.3.2 yields,

$$\langle E \rangle = \sum_i \langle \psi | i \rangle \varepsilon_i \langle i | \psi \rangle$$

After rearrangement we have,

$$\langle E \rangle = \sum_i \varepsilon_i |\langle i | \psi \rangle|^2$$

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

$$\langle E \rangle = \sum_i \varepsilon_i p_i \geq \varepsilon_0$$

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.

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