The Power of the Variational Method

1. Approximation Techniques

1.1. A Bit of Background

Anyone who has done enough quantum mechanics probably realizes that it is, more than anything else, the realm of analytically unsolvable problems. Due to the ubiquity of such quantum mechanical systems, humanity has, out of pure necessity, developped approximation techniques that allow us to very closely predict their behavior and evolution.

The techniques one most often encounters are the following :

- Time Independent Perturbation Theory
- Time Dependent Perturbation Theory
- The Variational Method

1.2. The Variational Method

The variational method is particularly fascinating since, unlike the other two techniques, it allows us to assign an upper bound to the ground-state energy without having access to solutions of the exact Hamiltonian of a closely related problem.

Thus, in the following paper, we will only attempt to demonstrate why the variational method works, and how it gives us an upper bound for the ground-state energy of the problem at hand.

2. Demonstration

Assume we have a system described by the Hamiltonian $\hat{H}$ (we will now drop the hat symbol for operators since no ambiguity shall arise, so $\hat{H}$ will be written as simply H from now on).

We define :

$$H' = \frac{\langle\psi'|H|\psi'\rangle}{\langle\psi'|\psi'\rangle} \tag{1}$$

where $|\psi'\rangle$ is an arbitrary ket that tries to emulate the true ground-state ket. One could think of it as a simple stand-in, a mathematical tool whose only purpose is to allow us to determine an upper-bound to our true ground-state energy that we shall call E_0[1].

To prove this, we define $|\psi\rangle$ as the true eigenstate of the original Hamiltonian H such that:

$$H|\psi\rangle = E_\psi|\psi\rangle$$

Following from the fact that the Hamiltonian H is an observable, these eigenstates form a complete orthonormal basis.

It is then trivial to see that one could use the closure relation that defines that same basis to express our emulating ket as :

$$|\psi'\rangle = \sum_{k=0}^{\infty}|\psi\rangle\langle\psi|\psi'\rangle \tag{2}$$

We then substitute 2 into 1, and we get :

$$H' = \frac{\left(\sum_{\psi=0}^{\infty}\langle\psi'|\psi\rangle\langle\psi|\right)H\left(\sum_{\psi=0}^{\infty}|\psi\rangle\langle\psi|\psi'\rangle\right)}{\left(\sum_{\psi=0}^{\infty}\langle\psi'|\psi\rangle\langle\psi|\right)\left(\sum_{\psi=0}^{\infty}|\psi\rangle\langle\psi|\psi'\rangle\right)}$$

[1] $|\psi'\rangle$ appears to serve an analogous purpose to the parameters we introduce in the Lagrange Multipliers method

$$= \frac{\sum_{\psi=0}^{\infty} \langle\psi|H|\psi\rangle\langle\psi'|\psi\rangle\langle\psi|\psi'\rangle}{\sum_{\psi=0}^{\infty} \langle\psi|\psi\rangle\langle\psi'|\psi\rangle\langle\psi|\psi'\rangle}$$

$$= \frac{\sum_{\psi=0}^{\infty} |\langle\psi'|\psi\rangle|^2 \ \langle\psi|H|\psi\rangle}{\sum_{\psi=0}^{\infty} |\langle\psi'|\psi\rangle|^2}$$

$$= \frac{\sum_{\psi=0}^{\infty} |\langle\psi'|\psi\rangle|^2 \ \left(E_\psi - E_0 + E_0\right)}{\sum_{\psi=0}^{\infty} |\langle\psi'|\psi\rangle|^2}$$

Finally, we obtain the following expression for our arbitrary Hamiltonian H' :

$$H' = \frac{\sum_{\psi=1}^{\infty} |\langle\psi'|\psi\rangle|^2 \ \left(E_\psi - E_0\right)}{\sum_{\psi=0}^{\infty} |\langle\psi'|\psi\rangle|^2} + E_0$$

Recall that, since E_0 is the ground-state energy, $E_\psi - E_0 > 0$. We can then confidently write :

$$H' > E_0$$

Thus, we have successfully found an upper bound for the true ground-state energy of the quantum mechanical system at hand, without necessarily having access to the Hamiltonian of an analogous system.