Variational Method in Quantum Mechanics

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Sometimes, we are interested in finding a bound on the ground state energy of a given system with Hamiltonian

$$H = H_0 + V(t), \tag{1}$$

where $V(t)$ is the perturbation to the known Hamiltonian H_0. This is especially useful if we don't know the exact solutions (eigenenergies and eigenstates) to the Hamiltonian H_0, which is required for using time-independent perturbation theory.

The variational method estimates the ground state energy E_0 by guessing a trial ground state wave function $|\tilde{0}\rangle$ and noting that

$$\bar{H} = \frac{\langle\tilde{0}|H|\tilde{0}\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \geq E_0. \tag{2}$$

The denominator $\langle\tilde{0}|\tilde{0}\rangle$ is there since $|\tilde{0}\rangle$ may not be normalized. Often we include a variational parameter λ into our trial wave function, and then choose the value of λ which minimizes $\bar{H}$ by solving for λ when

$$\frac{\partial \bar{H}}{\partial \lambda} = 0. \tag{3}$$

1 Dealing with a Discontinuity for $|x|$

We have had homework problems in the past where our trial wave function is

$$\psi(x) = \langle x|\tilde{0}\rangle = e^{\lambda|x|}. \tag{4}$$

Since the Hamiltonian includes the term

$$p^2 = \frac{d^2}{dx^2}, \tag{5}$$

we end up having to deal with the discontinuity at $x = 0$. This is done by splitting up the integral into three parts:

1. From $-\infty \to -\epsilon$
2. From $-\epsilon \to \epsilon$
3. From $\epsilon \to \infty$

and then taking the limit as $\epsilon \to 0$. I believe there is a problem of this form in chapter 5 of Sakurai, and there is a worked out solution on page $36 - 37$ of Kate's notes.