Exercise / We prove the variational principle.

(Source: Griffiths 8.1)

The variational principle states that the ground state energy E_0 of any system governed by a Hamiltonian H obeys

$$E_0 \leq \langle H \rangle,$$

where $\langle H \rangle = \langle \Psi | H | \Psi \rangle$ for any normalizable state $|\Psi\rangle$.

Proof

H is a Hermitian operator, so its eigenfunctions $\{|\Psi_n\rangle\}_n$ form a complete orthonormal set:

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle, \quad \langle \Psi_m | \Psi_n \rangle = \delta_{mn}.$$

We can then express an arbitrary normalizable state in this basis

$$|\Psi\rangle = \sum_n c_n |\Psi_n\rangle \implies$$

$$\langle \Psi | \Psi \rangle = \sum_{n,m} \langle \Psi_m | c_m^* c_n | \Psi_n \rangle = \sum_n |c_n|^2 = 1.$$

It follows that

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \sum_{m,n} \langle \Psi_m | c_m^* H c_n | \Psi_n \rangle =$$

$$\sum_{m,n} \langle \Psi_m | c_m^* c_n E_n | \Psi_n \rangle = \sum_n |c_n|^2 E_n \geq$$

$$\sum_n |c_n|^2 E_0 = E_0,$$

where we used the fact that $E_n \geq E_0$ for all n. Thus, we have shown

$$E_0 \leq \langle H \rangle$$

for any trial state. $\blacksquare$