Quantum Mechanics is Simple

One of the main reasons that classical problems can be hard on computers has a physical interpretation that if there is some energy function E, which is a function of classical variables $\mathbf{x}$, there can be many local minima $\partial E/\partial \mathbf{x} = 0$, which are not global minima. When the number of these local (but not global) minima gets infinitely large,[1] the classical problem is said to have (physical) *complexity.* In this problem, you will prove that quantum problems are *simple*: all local minima of the energy operator, defined on a wave function ψ in the natural way:

$$E[\psi] \equiv \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle},$$

are also global minima. For simplicity in this problem, we will focus on the case where the Hilbert space is finite dimensional, so that H is an $N \times N$ Hermitian matrix and $|\psi\rangle$ is just an N component complex vector, but the proof is more general and only relies on the fact that the Schrödinger equation is linear.

(a) Begin with the case $N = 2$. Argue that the most general two state Hamiltonian worth considering is

$$H = \epsilon \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Show that any local minimum of $E[\psi]$ for this Hamiltonian is also a global minimum. Give a geometric interpretation of the variational energy as a function of the point in the Hilbert space.

(b) Next, consider to general N. Show that any extremum of $E[\psi]$ occurs when ψ is an eigenvector of H.

(c) Combine the results of the previous two parts to prove that the only local minima of $E[\psi]$ are *global minima.*

This result has important consequences. If you are trying to find the ground state of a quantum mechanics problem on a computer, you don't have to worry about your variational algorithm getting stuck at a suboptimal solution – so long as you explore the whole phase space, the algorithm will easily find the ground state.

[1] One must excise from this definition a trivial infinity of minima, such as would occur if E was a constant function.