Quantum Mechanics and Computations

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Having analytically obtained an estimate for the critical points, we turn to the Schroedinger Wave Equation. We can turn the relation

$$H\psi = E\psi \tag{1}$$

into an eigenvalue problem using the finite difference method to represent the Hamiltonian operator as a vector.

To obtain our Hamiltonian vector, we first nondimensionalize the Hamiltonian operator,

$$H = \frac{\hat{p}^2}{2m} + \vec{V} \tag{2}$$

$$= -\frac{\hbar^2}{2m}\nabla^2 + \vec{V}. \tag{3}$$

We are only concerned about the r component of the ∇ operator, so this becomes

$$H = \frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\right] - \frac{c}{r}e^{-r/l}. \tag{4}$$

This can be nondimensionalized using the same constants from the nondimensionalized energy, becoming

$$H = \frac{c}{2\alpha}\tilde{H} = \frac{c}{2\alpha}\left[-\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{d}{d\rho}\right) - \frac{2}{\rho}e^{-\rho/\lambda}\right]. \tag{5}$$

The constant out front is the same one we pulled out of the energy, which allows us to restate (1) as

$$\tilde{H}\psi = \tilde{E}\psi.^1 \tag{6}$$

Before constructing the finite difference matrix to solve for $\tilde{E}$, we can simplify the with the substitution[2] $u(\rho) = \rho\phi(\rho)$. Plugging this into the above yields

[1] Using $\tilde{E}$ instead of e to avoid confusion with Euler's number.

[2] I should have a cite here.