Project 2:
Solving Schrödinger's equation for two electrons in a 3D harmonic oscillator well

Josh Bradt

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1 Introduction

A commonly studied system in physics is that of the electron confined in a potential well of some sort. This arises in, for example, the study of quantum dots, quantum computing, and other areas of solid-state physics.

Assuming spherical symmetry, we can write the radial part of Schrödinger's equation as follows for the confined electron in three dimensions:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r). \tag{1}$$

Here, $R(r)$ is the radial wave function of the electron, l is the angular momentum, $V(r)$ is the confining potential, and E is the energy. If we take the potential to be the three-dimensional harmonic oscillator potential,

$$V(r)=\frac{1}{2}m\omega^2r^2, \tag{2}$$

then the energies are known to be

$$E_{nl}=\hbar\omega\left(2n+l+\frac{3}{2}\right) \tag{3}$$

with quantum numbers $n=0,1,2,\dots$ and $l=0,1,2,\dots$.

Next, make the substitution $R(r)=(1/r)u(r)$ in (1) to find

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)u(r)+V(r)u(r)=Eu(r).$$