PHY 520: Group Project - Written Documentation
Steven Wallbrown, Henry Colburn, Bruce He, Otho Ulrich

We present descriptions of our models in three parts. In this document, the infinite square well and 1/r potential models are presented. The simple harmonic oscillator is described in word document, accompanying this submission. In each case, a model was built in mathematica that parallels the developments in "Introduction to Quantum Mechanics" [Griffiths] and Dr. Chris Crawford's course notes for the PHY 520 course at UK, 2017.

The states were easy to model without normalization. We found that normalizing the states was a difficult consideration. We were pleased to see the qualitative behaviour we expected, at least, and look forward to developing similar models more fully. The simple harmonic oscillator is plotted in 1d and 2d, and the infinite square well and 1/r potential solutions are plotted in 1d. Mathematica programs are included in this submission.

Modeling the infinite square well potential

The concept behind the simulation created is that of the infinite square well potential of a one-dimensional wave. The basics behind the idea is that a particle trapped in an area bordered by infinite potential must be composed of waves whose nodes correspond to the distance from one infinite potential barrier to another. The waves must be zero at the boundaries but are not required to have their derivatives be zero since there is no exponential decay of the wave, due to the infinite potential. Thus, the classical equation, $\sin(n\pi x/a)$ (where a is the well width and n is an integer) works for this situation where as the full quantum equation is not neccesary. This gives rise to the quantization of the energy levels so only discrete values are allowed. The program in Mathematica is designed so that up to three different waves can be plotted of different energy levels. The Y axis is the energy levels of the waves and the x axis is the width of the well. The program demonstrates the relationship between the number of nodes of a wave (entered in as n1, n2, and n3) and the energy levels associated with those waves. The simulation also draws attention to the spreading out of each successive wave from its predecessor in terms of separation energy, e.g. to go from n=5 to n=6 requires less energy input than n=100 to n=101. Within each wave function being plotted there is a horizontal line that represents the energy level of the wave that is on top of it. This is for a clearer representation of the energy level of the wave. The plotting range was also modified within each function so as to guarantee the plot would be large enough to fit up to the highest energy wave. With continued playing, the relationship between energy increases and node variation would become apparent to a user.

Modeling the 1/r potential - Hydrogen Atom

To model a quantum particle in a radial potential, we addressed the derivation of the wave function parallel with the development in Griffiths, pg. 145, and in Dr. Crawford's course notes, and some various online sources.

The potential V(r) = 1/r in spherical coordinates describes the system as having constants of motion in the angular coordinates theta and phi,

thus conserving angular momentum. Still, it admits an effective potential that includes a centrifugal factor,

$$V_{eff}(r) = V(r) + \hbar^2/2m\ l(l+1)/r^2.$$

The Schrodinger Equation with this potential may be solved using separation of variables. In this development, we focus on the radial wave function. The Schrodinger equation reads

$$-\hbar^2/2m\ d^2/dr^2\ \psi + [-1/r + \hbar^2/2m\ l(l+1)/r^2]\ \psi = E\ \psi.$$

$$[-1/r + \hbar^2/2m\ l(l+1)/r^2]\ \psi = E\ \psi + \hbar^2/2m\ d^2/dr^2\ \psi.$$

$$1/-E\ [-1/r + \hbar^2/2m\ l(l+1)/r^2]\ \psi = -\psi + \hbar^2/-2mE\ d^2/dr^2\ \psi.$$

$$[1/rE + \hbar^2/-2mE\ l(l+1)/r^2]\ \psi + \psi = \hbar^2/-2mE\ d^2/dr^2\ \psi.$$

We can introduce the variable $\kappa = \sqrt{(-2mE)}/\hbar$, giving

$$[1 + 2m/\hbar^2\kappa\ 1/\kappa r + l(l+1)/(\kappa r)^2]\ \psi = 1/\kappa^2\ d^2/dr^2\ \psi.$$

Set $\rho = \kappa r$, revealing $\rho_0 = 2m/\hbar^2\kappa$, which now gives

$$[1 + \rho_0/\rho + l(l+1)/\rho^2]\ \psi = d^2/d\rho^2\ \psi.$$

Note that by scaling ρ, we can translate this problem from the problem V(r) = 1/r to that of the hydrogen atom, with its specific radius. This is planned for later in the development.

Using an asymptotic breakdown, we can find the solution in three parts,

$\rho \to \infty$: $d^2/d\rho^2\ \psi = \psi$,
with solution $\psi(\rho) = A\ \exp(-\rho) + B\ \exp(\rho)$,
and since the second factor is not normalizable,
$\psi(\rho) = A\ \exp(-\rho)$.

$\rho \to 0$: $d^2/d\rho^2\ \psi = l(l+1)/\rho^2\ \psi$,
with solution $\psi(\rho) = C\ \rho^{l+1} + D\ \rho^{-l}$,
but $D\rho^{-l}$ disobeys normalizability, so
$\psi(\rho) = C\ \rho^{l+1}$.

The complete solution is then constructed assuming a power series v(ρ),

$$\psi(\rho) = A\ \exp(-\rho)\ C\ \rho^{l+1}\ v(\rho),$$

$$\text{where } v(\rho) = \sum_{j=0}^{\infty} c_j\ \rho^j.$$

The recursion relationship for the c_j coefficients is given by

$$c_{j+1} = \left\{ \frac{2(j + l + 1) - \rho_0}{(j + 1)(j + 2l + 2)} \right\} c_j,$$

where c_0 is normalized by total probability equal to one.

In general, this power series does result in unnormalizable states. There must be a maximum value of j, then, above which the coefficients are all zero. This jmax is related to the quantum numbers n and l by

$$j_{max} = n - l + 1.$$

Looking back at the recursion relationship, it becomes clear that

$$2(j + l + 1) - \rho_0 = 2n - \rho_0, \text{ and } \rho_0 = 2n.$$

This gives us a relationship between the principle quantum number n and the energy of a state n, recalling that the angular momentum is conserved and so the energy value does not rely on the quantum numbers l or m.

$$E_n = -\hbar^2\kappa^2/2m.$$

$$\kappa = 2m/\hbar^2\rho_0.$$

$$E_n = -2m/\hbar^2\rho_0{}^2 = -m/2\hbar^2n^2 = E_1/n^2, \; n = 1,2,3\ldots,$$
where $E_1 = -m/2\hbar^2$.

Actually, this is not an energy. The scaling factor bringing this to solutions of the hydrogen atom would make it an energy. It comes back to the units of V(r) = 1/r. This of course has units of energy, but what are the constants that make it that way? We've used no constants here. This should at least be $V(r) = E_0/r$, for some energy.

This reveals the dependence on the principle quantum number of the previous quanties,

$$\kappa = 2m/\hbar^2\rho_0 = a/n,$$
where $a = m/\hbar^2$ is the Scrodinger constant factor relating the action and mass of this system (or if scaled to the correct units, the inverse of the Bohr radius of the Hydrogen atom);

$$\rho = \kappa r = ar/n.$$

This is where it becomes obvious the scaling would be good, because here we would see that the form reveals r/(bohr radius).

The spatial wave function is defined by three quantum numbers n, l, and m, and as previously stated, can be solved by separation of various such that

$$\Psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\, Y_l^m(\theta,\phi),$$

where we have already found the radial function R,

$$R_{nl}(r) = 1/r \exp(-\rho)\, \rho^{l+1}\, v(\rho).$$

The model we've developed is nearly capable of handling the associated LaGuerre polynomials, but they become difficult to plot. So, for now, we focus on the radial function, only.

Substituting our new information back into the recursion relationship gives us the recursion in terms of the quantum numbers,

$$c_{j+1} = \left\{\frac{2(j + l + 1 - n)}{(j + 1)(j + 2l + 2)}\right\} c_j.$$

This is sufficient information to model the radial component of the wave function, except for normalizing the coefficient c_0. This is done using the expression of probability conservation

$$\int_0^\infty |R_{n\ell}|^2 \, r^2 \, dr = 1.$$

We want to simulate the hydrogen atom, where $V(r) \neq -1/r$, but instead $V(r) = -e^2/(4\pi\varepsilon_0)\ 1/r$. This changes some of our parameters, i.e.,

$\rho = \kappa r = r/an$ and $\rho_0 = m\ e^2/(2\pi\ \varepsilon_0\ \hbar^2\ \kappa)$,

where a now represents the Bohr Radius,

$a = 5.29 \times 10^{-2}$ nm.

The rest of the development is essentially the same.

In general, the normalization is given by

$$\left(\frac{(2/na)^3\ (n-l-1)!}{2n\ [(n+l)!]^3} \right)^{1/2}.$$

We will notate this normalization as α. If we also notate the generalized Laguerre polynomials of x as L[q,p](x), then our model is

$$\alpha \exp(-r/na)\ (2r/na)^l\ L[n-l-1,2l+1](2r/na)\ Y_\ell^m(\theta,\phi).$$

We have not plotted this, but here Y_ℓ^m refers to the spherical harmonics, which have the form (to within a normalization constant)

$Y_\ell^m(\theta,\phi) = \exp(\iota m\phi)\ P_\ell^m\ (\cos\theta)$,

where $P_\ell^m(x)$ are the Legendre Polynomials in x.

This model is implemented in mathematica, and will be presented to the Physics 520 class on Dec. 8, 2017.