Computational Assignment 1: Using the Laguerre Basis to get Hydrogen Energies and Radial Wavefuctions

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1 Problem 1

Solutions to the Schrodinger equation for the Hydrogen atom come in the separable form:

$$\Phi_{nlm}(\mathbf{r}) = \Phi_{nl}(r) * Y_l^m(\hat{\mathbf{r}}) \tag{1}$$

Where $\Phi_{nl}(r)$ are the spherically symmetric radially dependent parts of the wavefunction and $Y_l^m(\hat{\mathbf{r}})$ are the Spherical Harmonics, for the quantum numbers n,l and m, representing the principal, angular and magnetic quantum numbers.

These wavefunctions can be represented as:

$$\Phi_{nlm}(\mathbf{r}) = \Phi_{nl}(r) * Y_l^m(\hat{\mathbf{r}}) \tag{2}$$

Analytical solutions to the bound state radial part of the hydrogen atom are completely known, the first few relevant ones for the rest of this report follow:

n	l	$\Phi_{nl}(r)$
1	0	$2re^{-r}$
2	0	$\frac{r}{\sqrt{2}}(1-\frac{r}{2})e^{-r/2}$
2	1	$\frac{r^2}{\sqrt{24}}(1-\frac{2r}{3}+\frac{2r^2}{27})e^{-r/3}$
3	0	$\frac{2r}{\sqrt{27}}(1-\frac{2r}{3}+\frac{2r^2}{27})e^{-r/3}$
3	1	$\frac{8r^2}{27\sqrt{6}}(1-\frac{r}{6})e^{-r/3}$
4	1	$\frac{r^2}{64\sqrt{15}}(\frac{r^2}{4}-5r+20)e^{-r/4}$

If we choose a set of basis functions ϕ_j for $k = 1, 2, \ \ldots \ , \infty$ which form a complete basis on the Hilbert space, defined as:

$$\langle \mathbf{r}|\phi_j\rangle = \frac{1}{r}\phi_{k_j,l_j}(r)Y_{l_j}^{m_j}(\hat{\mathbf{r}}) \tag{3}$$

These basis function can be used to recover high order approximations to the true radial wavefunction through a sum over a finite number of the basis functions in the following way:

$$|\Phi_i\rangle = \sum_{j}^{N} c_j i \, |\phi_j\rangle \tag{4}$$

Which

1.1 Problem 2

INTRODUCE THESE IDEAS

Where the Real wavefunction can be recovered as a linear combination of all of these vectors:

$$|\Phi\rangle = \sum_{j} c_j \, |\phi_j\rangle \tag{5}$$

If we make this substitution into the Schrodinger equation:

$$\sum_{j} c_j \mathbf{H} \, |\phi_j\rangle = E \sum_{j} c_j \, |\phi_j\rangle \tag{6}$$

$$\sum_{j} c_j \, \langle\phi_i| \, \mathbf{H} \, |\phi_j\rangle = E \sum_{j} c_j \, \langle\phi_i|\phi_j\rangle \tag{7}$$

As a matrix equation then becomes:

$$\sum_{j} c_{ji} \mathbf{H_{ij}} = E_i \sum_{j} \mathbf{B_{ij}} c_{ji} \tag{8}$$

In the compute program this is performed over a finite basis N, thus we get:

$$\sum_{j}^{N} c_{ji} \mathbf{H_{ij}} = E_i \sum_{j}^{N} \mathbf{B_{ij}} c_{ji} \tag{9}$$