

# 1 Schrodinger Equation

The time-independent wavefunction,  $\psi$ , for any number of interacting electrons,  $N_e$ , can be computed by solving the time-independent Schrödinger Equation.

$$H\psi = E\psi \quad (1)$$

The Hamiltonian,  $H$ , under the Born-Oppenheimer approximation, consists of three terms. The kinetic energy,  $K$ , the external potential,  $V_{ext}$ , and the electron-electron interaction,  $V_{ee}$ . Assuming atomic units,  $\hbar = m_e = a_0 = e = 1$ , the Hamiltonian takes a relatively simple form.

$$H = K + V_{ext} + V_{ee} \quad (2)$$

$$K = \sum_{i=1}^{N_e} -\frac{\nabla_i^2}{2} \quad (3)$$

$$V_{ext} = V(x_1, x_2, \dots, x_D) \quad (4)$$

$$V_{ee} = \sum_{i=1}^{N_e} \sum_{j \neq i}^{N_e} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (5)$$

Each  $\mathbf{r}_i$  denotes a set of coordinates that describe the location of an electron in  $D$  dimensional space.

## 2 One Dimension

By restricting the systems of interest to one dimension, the external potential reduces to a function of one variable,  $x$ , and each electron only has a single coordinate,  $x_i$ .

$$V_{ext} = V(x) \quad (6)$$

$$V_{ee} = \sum_{i=1}^{N_e} \sum_{j \neq i}^{N_e} \frac{1}{|x_i - x_j|} \quad (7)$$

It also simplifies the kinetic term to a sum across single variable second derivatives.

$$K = \sum_i^{N_e} -\frac{1}{2} \frac{d^2}{dx_i^2} \quad (8)$$

### 3 Delta Basis Functions

Now, to solve the time-independent, one dimensional, Schrödinger Equation a representation of the wavefunction is needed. Commonly, this representation is a sum over a set of a number of basis functions,  $N_B$ , where each basis function is a product state of single particle functions,  $f(x_i)$ .

$$\psi(x_i, x_{i+1}, \dots, x_{N_e}) = \sum_{j=1}^{N_B} c_j \prod_{i=1}^{N_e} f(x_i) \quad (9)$$

This allows for the calculation of the Hamiltonian in the chosen representation and its diagonalization leading to the coefficients of our basis functions,  $c_j$ .

While there are many choices for the single particle functions in 1D, such as the eigenfunctions of the particle in a box or the harmonic oscillator. The simplest and most intuitive choice for this representation would be delta functions.

$$\delta(x) = \begin{cases} 1, & \text{if } x = 0 \\ 0, & \text{otherwise} \end{cases} \quad (10)$$

By employing delta functions in this manner each included basis function can be viewed as the inclusion of another grid point with a magnitude of one. Then, the solved coefficients are the proper values of the full wavefunction on each grid point. The wave functions are being solved on a real space grid and the number of basis functions is the same as the number of grid points,  $N_x$

### 4 Three Particles 1D box

Moving to three particles the wavefunction is a product of three one particle functions running over indices  $\{(i = 1, 2, \dots, N_x), (j = 1, 2, \dots, N_x), (k = 1, 2, \dots, N_x)\}$ .

$$\psi(x_1, x_2, x_3) = \delta(x_1 - \Delta i) \delta(x_2 - \Delta j) \delta(x_3 - \Delta k) \quad (11)$$

To calculate the Hamiltonian for this wavefunction we need to run over all possible combinations of  $i$ ,  $j$ , and  $k$ . The total number of possible combinations in this case is  $N_x^3$  leading to a Hamiltonian of size  $(N_x^3, N_x^3)$  assuming even grid spacing of  $\Delta$ .

To obtain this matrix three corollary indices  $p$ ,  $q$ , and  $r$  need to be introduced and all six indices need to be reduced to two ordered indices.

$$n = (p - 1) * N_x^2 + (q - 1) * N_x + r \quad (12)$$

$$m = (i - 1) * N_x^2 + (j - 1) * N_x + k \quad (13)$$

Each element of the Hamiltonian can now be written as:

$$H_{n,m} = \int_0^L \int_0^L \int_0^L \psi_{p,q,r}(x_1, x_2, x_3) \mathbf{H} \psi_{i,j,k}(x_1, x_2, x_3) dx_1 dx_2 dx_3 \quad (14)$$

$$H_{n,m} = K_{n,m} + V_{ext,n,m} + V_{ee,n,m} \quad (15)$$

A byproduct of the reduction to two indices is that the each pair of correlated delta functions becomes a Kronecker delta of their corollary indices.

$$\delta_{i,j} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases} \quad (16)$$

$$\psi p, q, r(x_1, x_2, x_3) \psi_{i,j,k}(x_1, x_2, x_3) = \delta_{p,i} \delta_{q,j} \delta_{r,k} \quad (17)$$

As a result the interaction potential and external potentials become diagonal matrices.

$$V_{ee,n,m} = \frac{\delta_{n,m}}{\Delta} \left( \frac{1}{|i-j|} + \frac{1}{|i-k|} + \frac{1}{|j-k|} \right) \quad (18)$$

$$V_{ext,n,m} = \delta_{n,m} V(\Delta(k-1)) \quad (19)$$

The kinetic matrix is then a highly sparse banded matrix with bands along the main diagonal and the off diagonals at an offset of positive and negative one,  $N_x$ , and  $N_x^2$ .

$$\begin{aligned} K_{n,m} = & -\frac{1}{2\Delta^2} \{ \delta_{q,j} \delta_r, k (\delta_{p,i-1} - 2\delta_{p,i} + \delta_{p,i+1}) \\ & + \delta_{p,i} \delta_{r,k} (\delta_{q,j-1} - 2\delta_{q,j} + \delta_{q,j+1}) \\ & + \delta_{q,j} \delta_{p,i} (\delta_{r,k-1} - 2\delta_{r,k} + \delta_{r,k+1}) \} \end{aligned} \quad (20)$$

## 5 Soft-Coulomb

The Coulomb interaction as defined in previous sections can leads to singularities in one-dimensions which are impossible to solve with normal methods. Thus this work will employ a Soft-Coulomb interaction.

$$V_{sc} = \sum_{i=1}^{N_e} \sum_{j \neq i}^{N_e} \frac{1}{\sqrt{|x_i - x_j|^2 + a^2}} \quad (21)$$

The interaction is soft because the parameter  $a$  smooths out the Coulomb interaction as it grows larger thus removing the singularity. The form of Soft-Coulomb interaction is exactly the same as the normal interaction except for the location of the grid spacing term.

$$\begin{aligned} V_{sc,n,m} = & \delta_{n,m} \left( \frac{1}{\sqrt{|i-j|^2 \Delta^2 + a^2}} \right. \\ & + \frac{1}{\sqrt{|i-k|^2 \Delta^2 + a^2}} \\ & \left. + \frac{1}{\sqrt{|j-k|^2 \Delta^2 + a^2}} \right) \end{aligned} \quad (22)$$

## 6 Code

The code itself is fairly simple. The interaction energy matrix is placing a single vector  $N_x^3$  elements in length along the main diagonal of a scipy sparse matrix. Where, the main diagonal is calculated with three loops over the indices in eq (22). Next, the external potential is repeated  $N_x^2$  times making another vector consisting of  $N_x^3$  elements. Which is then summed into the main diagonal of Hamiltonian. The external potential can be made into it's own sparse matrix and then added to the kinetic and interaction or added into either the interaction or kinetic matrix on construction. This codes adds it along the main diagonal of the kinetic matrix upon construction.

Finally, the kinetic matrix is constructed as numpy diagonal matrix. The main diagonal of the matrix is  $N_e/\Delta^2$  and all other non-zero elements are  $-\frac{1}{2\Delta^2}$ . The most complicated part of the code is the fact that the off-diagonal bands contain elements that are zero. This requires that the off main diagonals need to be padded with zeros so that vectors are placed in the correct positions in the final kinetic matrix.

After the construction is done all that is required is diagonalizing the Hamiltonian. This code employs scipy's sparse hermitian eigensolver because the matrix is highly sparse and, if not too many grid points are wanted, small enough that ARPACK methods can be used straight out of the box.