

# Neutral Atom Solver

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## 1 Units

This code uses Hartree units where  $\frac{\hbar^2}{m_e} = e = 4\pi\epsilon_0 = 1$ .  $m_e$  is the mass of the electron

## 2 Grids

### 2.1 Uniform Grid

### 2.2 Exponential Grid

### 3 Second Order Differential Equation Solver

This section focus on solving two differential equations: Schrödinger's equation for one dimensional systems (including radial potentials for DFT atomic calculations), and Poisson's equation, we are then interested on numerically solving equations of the form: be written as:

$$\frac{d^2y}{dx^2} = f(x)y + g(x) \quad (1)$$

The first step to numerically solving this equation is by rewriting it as a system of linear differential equations such that  $y(x) \rightarrow y^0(x)$ ,  $\frac{dy(x)}{dx} \rightarrow y^1(x)$  such that equations 1 became:

$$\begin{cases} \frac{dy^0}{dx} = y^1(x) \\ \frac{dy^1}{dx} = f(x)y^0(x) + g(x) \end{cases} \quad (2)$$

This system of equations can be solved with method like Runge-Kutta order 4 and/or predictor corrector Adams-Moulton order 4.

To numerically solve the equations 2 the system must be translated into discrete sets of values. First by discretizing the space, into a grid of  $N$  values such that  $x_i$  is the value of the grid at position "i". The functions are also discrete  $f_i \rightarrow f(x_i)$  stands by evaluating a function  $f$  on the "i" position of the grid. And "h" stands for the delta between to consecutive points on the grid  $h = x_{i+1} - x_i$ , the grid points are not necessarily uniformly distributed. The objective is to find the  $N$  values of  $y$  over the grid, for a numerical solution the values of  $y(x_1)$  and  $y(x_2)$  must be known.

#### Runge-Kutta order 4

This subsection describes how a function (RK4) utilizes the Runge-Kutta order 4 method to produce the values  $y^0(x_{i+1})$ , and  $y^1(x_{i+1})$ .

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h ← (xi+1 - xi)
y0 ← y0(xi)
y1 ← y1(xi)
f̄ ← [f(xi), f(xi+1)]
ḡ ← [g(xi), g(xi+1)]
k01 = h * y1
k11 = h * (f̄[1] * y0 + ḡ[1])
k02 = h * (y1 + 0.5 * k11)
k12 = h * (0.5 * (f̄[1] + f̄[2]) * (y0 + 0.5 * k01) + 0.5 * (ḡ[1] + ḡ[2]))
k03 = h * (y1 + 0.5 * k12)
k13 = h * (0.5 * (f̄[1] + f̄[2]) * (y0 + 0.5 * k02) + 0.5 * (ḡ[1] + ḡ[2]))
k04 = h * (y1 + k13)
k14 = h * (f̄[2] * (y0 + k03) + ḡ[2])
y0(xi+1) = y0 +  $\frac{1}{6}$  * (k01 + 2 * k02 + 2 * k03 + k04)
y1(xi+1) = y1 +  $\frac{1}{6}$  * (k11 + 2 * k12 + 2 * k13 + k14)
return [y0(xi+1), y1(xi+1)]

```

#### Predictor Corrector Method Adams-Moulton Orders 4 and 5

Description of the predictor corrector Adams-Moulton (PCAM4) function implementation, the PCAM4 the integration routine produces  $y^0(x_i), y^1(x_i)$

$$\begin{aligned}
h &\leftarrow (x_i - x_{i-1}) \\
\bar{y}^0 &\leftarrow [y^0(x_{i-4}), y^0(x_{i-3}), y^0(x_{i-2}), y^0(x_{i-1})] \\
\bar{y}^1 &\leftarrow [y^1(x_{i-4}), y^1(x_{i-3}), y^1(x_{i-2}), y^1(x_{i-1})] \\
\bar{f} &\leftarrow [f(x_{i-3}), f(x_{i-2}), f(x_{i-1}), f(x_i)] \\
\bar{g} &\leftarrow [g(x_{i-3}), g(x_{i-2}), g(x_{i-1}), g(x_i)] \\
y_{prediction}^0 &= \bar{y}^0[4] + \frac{h}{24} * (55 * \bar{y}^1[4] - 59 * \bar{y}^1[3] + 37 * \bar{y}^1[2] - 9 * \bar{y}^1[1]) \\
y_{prediction}^1 &= \bar{y}^1[4] + \frac{h}{24} * (55 * (\bar{y}^0[4] * f[4] + g[4]) - 59 * (\bar{y}^0[3] * f[3] + g[3]) + 37 * (\bar{y}^0[2] * f[2] + g[2]) - 9 * (\bar{y}^0[1] * f[1] + g[1])) \\
y_{corrector}^0 &= \bar{y}^0[4] + \frac{h}{24} * (9 * y_{prediction}^1 + 19 * \bar{y}^1[3] - 5 * \bar{y}^1[2] + 1 * \bar{y}^1[1]) \\
y_{corrector}^1 &= \bar{y}^1[4] + \frac{h}{24} * (9 * (y_{prediction}^0 * f[4] + g[4]) + 19 * (\bar{y}^0[3] * f[3] + g[3]) - 5 * (\bar{y}^0[2] * f[2] + g[2]) + 1 * (\bar{y}^0[1] * f[1] + g[1]))
\end{aligned}$$

### 3.1 Schrödinger's equation

The time independent Schrödinger equation:

$$-\frac{1}{2}\nabla^2\Psi(\vec{r}) + V(r)\Psi(\vec{r}) = E\Psi(\vec{r}) \quad (3)$$

Assuming a solution of the form:

$$\Psi(\vec{r}) = \frac{u(r)Y_m^l}{r} \quad (4)$$

Where  $Y_m^l$  are the spherical harmonics such that after substituting equation 4 into equation 3, we get a radial Schrödinger equation of the form:

$$-\frac{1}{2}\frac{d^2u(r)}{dr^2} + \frac{l(l+1)u(r)}{2r^2} + V(r)u(r) = Eu(r) \quad (5)$$

Now introduce an effective potential that contains external potential, exchange, correlation, hartree, and angular

$$V_{effe} = V_{angu}(l, r) + V_{ext}(*parameters, r) + V_{hart}(\rho, r) + V_{exch}(\rho, r) + V_{corr}(\rho, r) \quad (6)$$

Rearranging terms equation 5 became:

$$\frac{d^2u(r)}{dr^2} = 2(V_{effe} - E)u(r) \quad (7)$$

And equation 7 has the form of equation 1 with  $f = 2(V_{effe} - E)$ ,  $g = 0$ , and  $y = u$