1D DFT

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The code is a simple one-dimensional SCF Kohn-Sham DFT code using periodic boundary conditions. I've used a plane-wave basis set of complex exponentials, $\phi_n = \frac{1}{\sqrt{L}} e^{i2\pi nx/L}$.

The KS Hamiltonian is contructed in the following way.

1 Kinetic contribution

$$T_{ij} = \langle \phi_i | \hat{T} | \phi_j \rangle = -\frac{1}{2} \int \phi_i^* \frac{d^2}{dx^2} \phi_j dx = \frac{1}{2} k_j^2 \delta_{ij}$$

Where $k = \frac{2\pi n}{L}$.

2 External contribution

$$V_{ij}^{ext} = \int \phi_i^* v(x) \phi_j dx$$

Where $v(x)$ is our external potential.

3 Hartree

The one dimenstional Poisson equation is, $\frac{d^2 V_H(x)}{dx^2} = -\rho(x)$, and we define in fourier space,

$$V_H(x) = \sum_q \tilde{V}_q e^{iqx}$$

$$\rho(x) = \sum_q \tilde{\rho}_q e^{iqx}$$

Combining, we get $\tilde{V}_q = \frac{\tilde{\rho}_q}{q^2}$ for $q \neq 0$, $\tilde{V}_0 = 0$.

The matrix elements are then,

$$(H_H)_{ij} = \frac{1}{L} \int e^{-ik_i x} \sum_q (\tilde{V}_q e^{iqx}) e^{ik_j x} dx = \frac{1}{L} \sum_q \tilde{V}_q \int e^{(k_j - k_i + q)x} dx$$

The only surviving terms are those with $q = k_i - k_j$. So we have for $k_i \neq k_j$,

$$(H_H)_{ij} = \tilde{V}_{k_i - k_j} = \frac{\tilde{\rho}_{k_i - k_j}}{(k_i - k_j)^2}.$$

$(H_H)_{ij} = 0$ for $k_i = k_j$.

4 Exchange

The 1D exchange functional I found online was $\epsilon_x = -\frac{\pi}{4}\rho(x)$, which gives a potential of $V_{ex} = -\frac{\pi}{2}\rho(x)$.

I have not implemented correlation yet as I don't know what's a good 1d correlation functional to use.