Computational Physics
Ex. 12 – DFT solver

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The exercise was done by modifying the provided Matlab code. The solver is implemented in `DFT_solver.m`. The script `run_DFT_solver.m` was used to run the solver and plot the results.

(a) The resulting electron density for $M = 1$ nucleus and $N = 3$ electrons is shown in Fig. **??**. The normalization of the solver seems to be correct as $\int \rho(x)\,\mathrm{d}x = 3$, as it should be since the normalized basis functions ϕ_i should satisfy

$$\int_{\infty}^{\infty} \rho(x)\,\mathrm{d}x = \int_{\infty}^{\infty} \sum_{i=1}^{3} |\phi_i(x)|^2\,\mathrm{d}x = \sum_{i=1}^{3} \int_{\infty}^{\infty} |\phi_i(x)|^2\,\mathrm{d}x = \sum_{i=1}^{3} 1 = 3. \tag{1}$$

The resulting electron density seems to be well contained within the potential well of the nucleus, which seems plausible.

(b) The system with two nuclei ($M = 2$) and six electrons ($N = 6$) was set up and the DFT solver was run at varying inter-nucleus separations Δx. The total energy of the system as a function of the separation is shown in Fig. **??**. From the plot, we can clearly see that the total energy is minimized by $\Delta x \approx 0.5$, indicating the presence of simple chemical bonding in our DFT system. The electron density for the energy-minimizing separation is plotted in Fig. **??**, along with the locations of, and the external potential caused by the two nuclei.

(c) About 8 hours in all.