

Implementation of Filter Matrix Diagonalisation in CP2K

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Introduction

In normal ab initio Density Functional Theory (DFT) [1] calculations, we minimise the total energy of the system with respect to electron density $\rho(\mathbf{r})$. One way of solving the problem requires the solution to the generalised eigenvalue problem:

$$\mathbf{H}\psi_n = E_n \mathbf{S}\psi_n$$

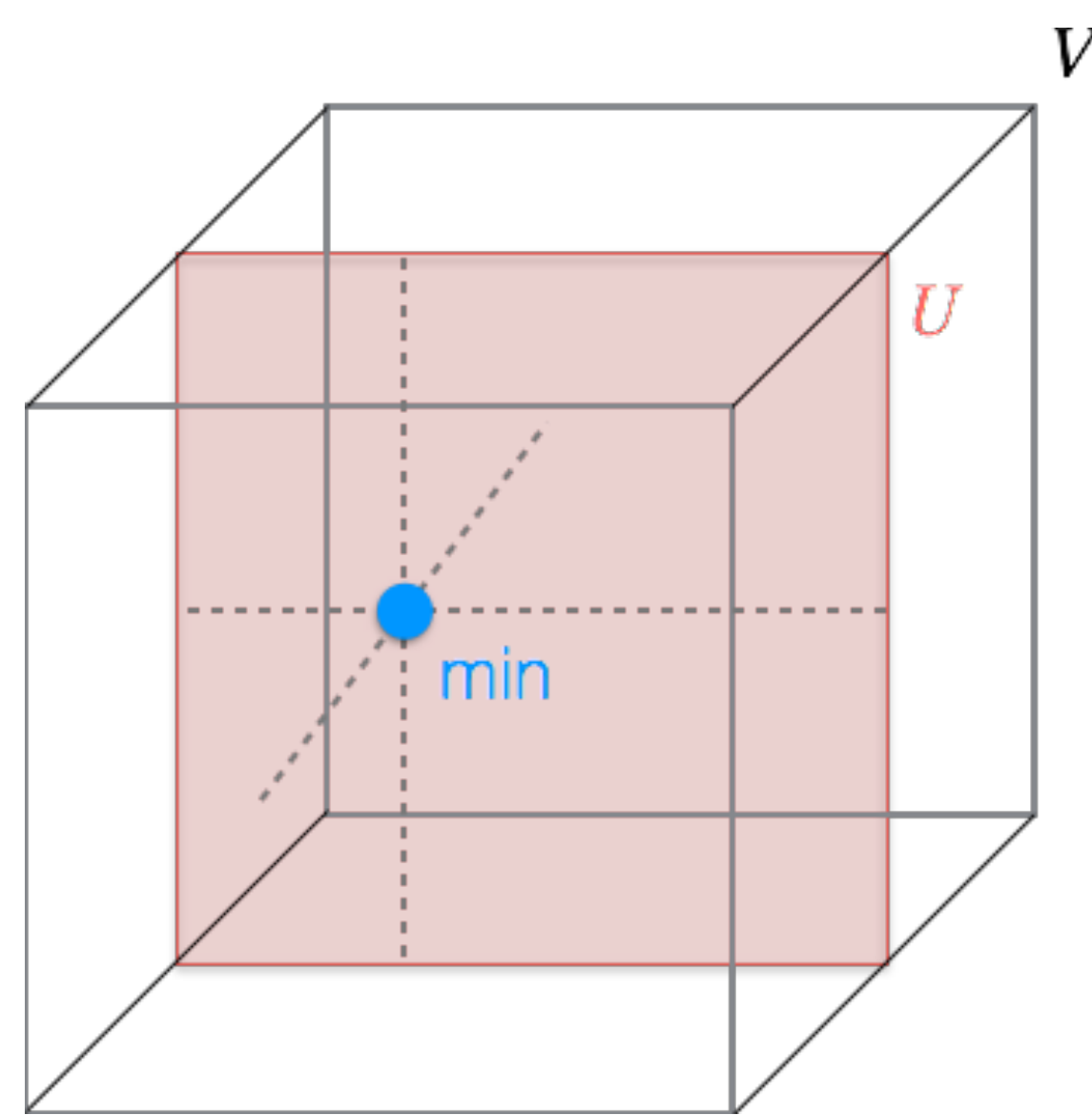
This approach allows smearing and is generally more stable than others in dealing with systems with small band gaps, such as metallic substances. However, diagonalisation is an $\mathcal{O}(N^3)$ problem, which means the calculation will become prohibitively expensive for large metallic systems. But CP2K [2,3] currently is a gamma-point only code, so accurate simulations of metallic systems usually require a large simulation cell.

A way thus has to be found to try to reduce the computational cost of solving the diagonalisation problem while not sacrificing accuracy. A method introduced by Rayson and Briddon [4] allows one to achieve this goal by dynamically projecting the eigenvalue problem into a space spanned by an optimised set of minimum basis functions, which dramatically reduces the problem size.

Need for Dynamic Optimisation

Assume the minimum energy is in the space spanned by the original basis functions (V).

U is the subspace spanned by a minimum basis set.



If the minimum basis is optimised at the beginning of the calculation, then if the atoms move or the electronic structure changes during the calculation, the minimum energy point while moving within V , will likely to move out of U .

Thus to find the same minimum energy, the minimum basis must be optimised at every SCF point, so that it keeps up with the movement of the ground state point.

Constructing New Basis

Assumptions:

1. At ground state, the energy of the partial system surrounding each atom should also be near their respective minimum
2. A new reduced sized basis for each atom can be constructed, still centered around each atom

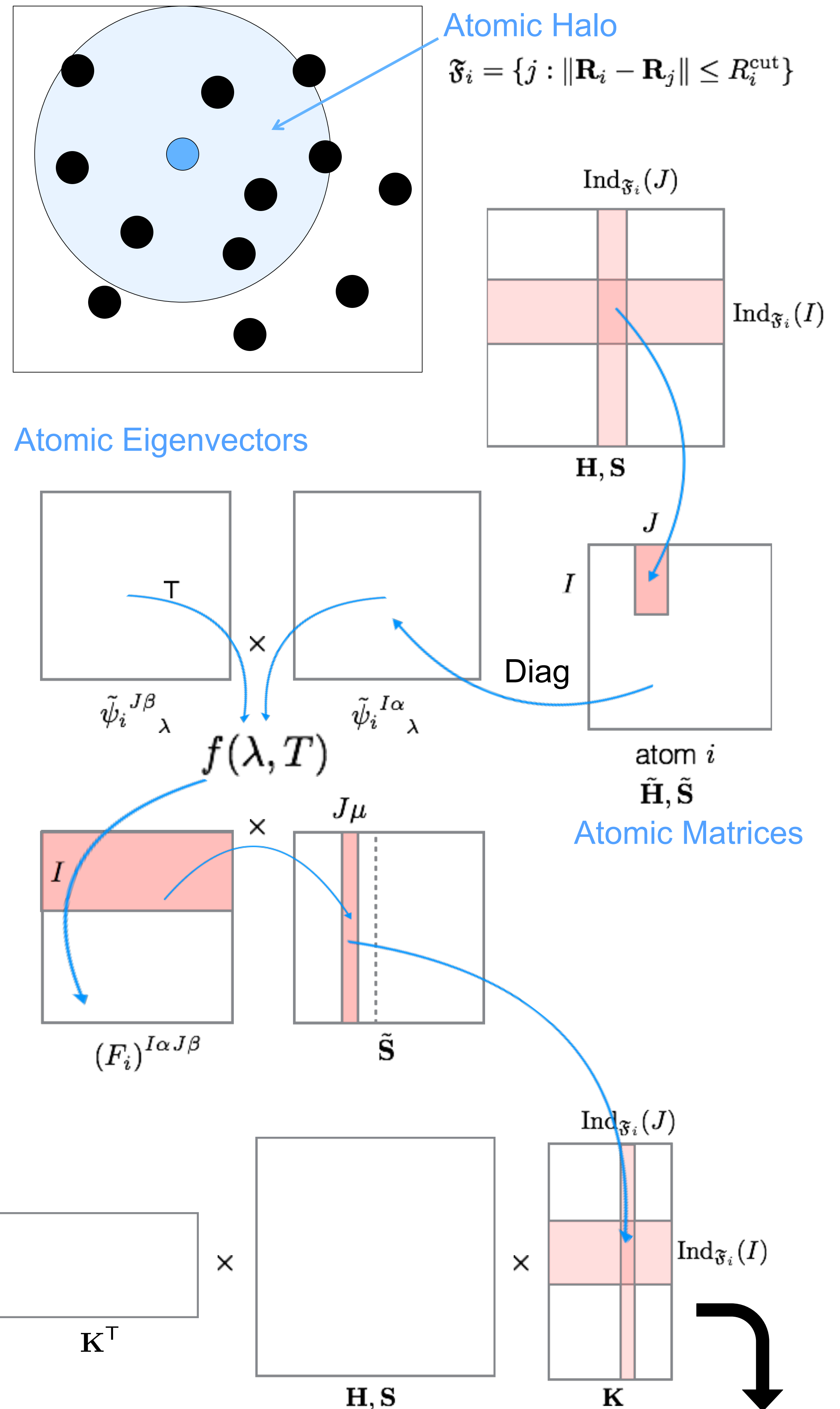
References

[1] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965)

[2] J. VandeVondele, et al., Comput. Phys. Commun. 167, 103 (2005)

[3] <http://www.cp2k.org>

[4] Rayson and Briddon, Phys. Rev. B 80, 205104 (2009)



Overall Scheme of Implementation

