Speeding up the ground-state Hamiltonian application in real space

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An implementation of the non-local potential in real space will be presented. This implementation is based on the well-known work of King-Smith *et al* [1]. We will show what are the necessary modifications in the code to achieve this, what approximations are introduced, and what is the expected numerical precision for this kind of calculation.
We have also explored some ways to improve the initial method, releasing degrees of freedom in optimizing the parameters.
The main application of this development lies in Molecular Dynamics calculations.

References

[1] R. D. King-Smith, M. C. Payne, and J. S. Lin. Phys. Rev. B 44, 13063 (1991).