A perturbation-method-based post-processing for the planewave discretization of Kohn–Sham models

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In order to determine the electronic structure of a molecular system, one often needs to solve a nonlinear eigenvalue problem. The numerical resolution of such a problem relies on a discretization, for example Fourier series, also called planewaves, that are often used when the system is a crystal. The quality of the discrete eigenvalues and eigenfunctions mostly depends on the grid size, hence on the number of degrees of freedom of the discrete space that, in turn, impact the cost of the computation, in a nonlinear way (e.g. quartic).

In this poster, a perturbation theory is used to post-process the approximate eigenvalues and eigenfunctions of a nonlinear eigenvalue problem, in a periodic setting [1][2]. This post-processing is based upon the fact that the exact solution can be interpreted as a perturbation of the approximate solution, allowing us to compute corrections in order to increase the accuracy of both the eigenvalues and eigenfunctions.

Practically, a first computation is done on a coarse grid at a rather low cost. Then the obtained eigenfunctions and eigenvalues are corrected on a fine grid also at very low cost, the computations involving only residual computations and FFT's. The quality of the corrected quantities is, after the postprocessing, comparable to the result of a full computation on the fine grid.

Theoretical estimates certify an increased convergence rate in the asymptotic convergence range. Numerical results confirm the low computational cost of the post-processing and show that this procedure improves the energy accuracy of the solution, in a substantial way, even in the pre-asymptotic regime which comprises the target accuracy of practitioners.

Références

[1] Eric Cancès, Geneviève Dusson, Yvon Maday, Benjamin Stamm, Martin Vohralík, *A perturbation-method-based a posteriori estimator for the planewave discretization of nonlinear Schrödinger equations*, C. R. Math. Acad. Sci. Paris 352 (2014), 941-946.

[2] Eric Cancès, Geneviève Dusson, Yvon Maday, Benjamin Stamm, Martin Vohralík, *A perturbation-method-based post-processing for the planewave discretization of Kohn–Sham models*, Journal of Computational Physics 307 (2016) 446-459.

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