A posteriori error analysis of a linear Schrödinger type eigenvalue problem for atomic centered discretizations

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In this poster, we present a first a posteriori error analysis for variational approximations of the ground state eigenpair of a linear Schrödinger type eigenvalue problem for systems with one electron and M atoms, more precisely of the form $Hu = \lambda u$, $H = -\Delta + \sum_{i=1}^{M} V_i + \sigma$, $\|u\|_{L^2} = 1$, with boundary conditions in one dimension. Denoting by (u_N, λ_N) the variational approximation of the ground state eigenpair (u, λ) based on a Gaussian discretization centered on atoms, we provide a posteriori estimates of the error in the energy norm $\|u - u_N\|_H$, when N goes to infinity. We introduce the residual of the equation and we decompose it into M residuals characterizing the error localized on atoms. It is shown that the bound can be expressed in terms of the dual "local" norms induced by the radially symmetric operators $H_i = -\Delta + V_i + \sigma_i, i = 1, \ldots, M$ centered on atoms. Such bound is fully computable as soon as an estimate on the dual local norms of the local residuals is available, which is obtained by performing a spectral decomposition of the bounded operators H_i of Hydrogen-like atoms. Finally, we provide numerical illustration of the performance of such a posteriori analysis on test cases.

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