

Abstract Submitted
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Quantum Perturbation Theory in $O(N)$: Ab initio response theory for nanomaterials ANDERS NIKLASSON, Theoretical Division, Los Alamos National Laboratory — One of the main obstacles in predicting the electronic properties of complex nanomaterials directly from fundamental theory is the enormous computational complexity involved in solving the equations governing the quantum mechanical response to an external perturbation. We have recently introduced an orbital-free quantum perturbation theory based on perturbed spectral projections of the Hamiltonian. It gives the density matrix and its response upon variation of the Hamiltonian by quadratically convergent recursions. The approach is surprisingly simple and efficient. It allows treatment of both embedded quantum subsystems and response functions. The computational cost scales linearly with the systems size N and for local perturbations it scales linearly with the size of the perturbed region $O(N_{\text{pert}})$, i.e. as $O(1)$ with the total system size. Traditional textbook perturbation theory based of wave function or Green's function formalism can be replaced by a quadratically convergent explicit recursion that gives the expansion terms of expectation values to any order. Connecting and disconnecting individual weakly interacting quantum subsystems can be performed by treating off-diagonal elements of the Hamiltonian as a perturbation. This should be highly useful in nanoscience for connecting quantum dots, surfaces, clusters and nanowires, where the different parts can be calculated separately.

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