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Fast Integral method for the calculation of Hartree and Exchange terms in DFT and TDDFT[1] MICHAEL ZUZOVSKI, AMIR BOAG, AMIR NATAN, Dept. of Physical Electronics, Tel-Aviv University, Israel — The Hartree and Exchange terms can become a computational intensive task in DFT and TDDFT calculations of large structures. Existing methods use either iterative solvers such as conjugate gradient or multi-grid methods or use FFT for the calculation of those terms via the solution of the Poisson equation. With iterative solvers, the problem of setting the boundary conditions is often time consuming by itself as approximations such as the multipole expansion might not converge easily for structures with high aspect ratio. With FFT one needs to use a larger box for the calculation of finite systems. We present an alternative integral method to calculate the Hartree and Exchange terms in DFT and TDDFT. We first describe the algorithm and show that it has O(N) scaling for elongated structures. We then show some examples of long 1D chains ground state and time dependent calculations that use this algorithm. Finally we discuss some possible applications for more advanced functionals that include the Fock exchange or screened exchange.

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