Truncation Algorithms for One-Dimensional Lattice Sums of Coulomb Integrals

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Over the past several years we have made substantial progress in developing an approach for density-functional electronic structure calculations on quasi-one-dimensional nanostructures with helical symmetry. In this talk we discuss the use of multipole-expansion methods for allowing efficient truncation of long-range Coulomb integral lattice summations. In particular, we discuss the use of polylogarithms and known computational algorithm for the efficient evaluations of these functions—in conjunction with extended precision computational routines—to allow the implementation of computational efficient methods for accurate evaluate of these lattice sums.