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A NEW ERI SCHEME IN QFMM

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As one of our on-going developments of linear or low scaling quantum theories, new ERI(Electron Repulsion Integral) scheme have been established that can be tightly integrated into the QFMM(Quantum Fast Multipole Method) code. As a result, a significant performance improvement is expected. The basic formulas is based on the combination of Fourier transformation and multipole expansions. In addition, a new direct determination of multipole moments of Cartesian Gaussian functions in Spherical polar coordinates, which significantly improves linear scaling performance, is also presented.
Theses developments will eventually enable us to perform *ab initio* studies of nano-size materials.