Local and non-local density fitting in periodic methods

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Density fitting (resolution of the identity) approximation [1] is routinely used in molecular electronic structure methods, in order to speed up evaluation of 4-index integrals, which are factorized into products of 3- and 2-index ones. In the periodic context, this technique cannot be straight-forwardly applied due to the infinite nature of the systems. We discuss the possible schemes for periodic density fitting, namely longe-range reciprocal-space [2], short-range direct-space [3] and combined [3,4] treatment. The density fitting is employed within the periodic local MP2 and CIS methods.

Literature:

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