The Spectral Ewald method for singly periodic Coulomb potentials

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A fast and spectrally accurate method is presented to efficiently compute the three dimensional Coulomb potential with periodicity in one direction. The derived algorithm is developed based on the framework of FFT-based methods using the so-called Ewald summation formula. In the periodic direction, a Fourier series is obtained which is computed effectively using FFTs. In the non periodic directions, however, Fourier integrals appear and the grid has to be oversampled to be able to use the FFT.

It is shown that to approximate the integrals accurately, the grid has to be upsampled by a factor of four in each non-periodic direction, making the grid 16 times larger. However, we show that upsampling is only needed for modes with small wave numbers in the periodic direction. For the zero wave number, the Fourier integral become singular, and this case must be considered separately. Here, we effectively need to solve a free-space Poisson equation in two dimensions. To do this, we make use of a very recent idea of Vico et al. by which we again can use FFTs to solve this problem. It fits directly into our framework, albeit requiring a different upsampling factor for this zero mode. We can hence unify the treatment of all modes, and construct an adaptive 3D FFT to apply different upsampling rates locally. With this technique, the total runtime is significantly reduced compared to full upsampling while the spectral accuracy is still preserved.

We show that the cost of computing this singly periodic potential is only marginally larger than the cost of computing the potential for a triply periodic system, where no upsampling is needed. We numerically compare our algorithm to the only previously existing algorithm and show that our method is competitive in terms of computational time and is more efficient in terms of memory consumption.