Fast Fourier Transformation and Spin Projection

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The evaluation of electronic matrix elements over a spin-independent many-electron Hamiltonian is considered. Using a spin adapted basis of configuration state functions, this evaluation is a complicated task.

Applying fast fourier transformation over a group /1,2/, we show how compact and efficient algorithms for this task may be obtained. Limiting to the case of the symmetric group here, we explain possible extensions to other groups reflecting molecular or particle symmetries. The fast fourier transformation approach is compared with the well established methods like the symmetric group approach or projection techniques.

/1/ M. Clausen, U. Baum, *Fast Fourier Transforms*, 1993

/2/ D. Maslen, D. Rockmore, in *Dimacs Series in Disc. Math. and Comp. Sci.* **28**, 1995, 138–238