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Towards a Fast Fourier Transform for Spherical Gauss-Laguerre Basis Functions

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Spherical Gauss-Laguerre basis functions (i.e., normalized functions of the type $\exp(-r^2/2)r^l L_{n-l-1}^{l+1/2}(r^2)Y_{lm}(\vartheta,\varphi)$ of order $n \in \mathbb{N}$ and degrees $l = 0, ..., n-1$, $|m| \leq l$; Y_{lm} being the spherical harmonics) are used extensively e.g. in molecular dynamic simulations, as well as in computational quantum mechanics in general. However, to the present, there is no reliable algorithm available to compute the Fourier coefficients of a function with respect to spherical Gauss-Laguerre (SGL) basis functions in a fast way. In this work, we combine the results of [1] and [2] to derive an SGL sampling theorem that permits an exact computation of the SGL Fourier expansion of a given function, provided that the expansion is of order at most $N \in \mathbb{N}$. The fact that the SGL basis functions satisfy a three-term recurrence relation in the order n then allows us to use the techniques of [3] to state a fast SGL Fourier transform. This algorithm has complexity $\mathcal{O}(N^3 \log^2 N)$, instead of the complexity $\mathcal{O}(N^6)$ associated with the direct approach, and is currently investigated for its performance.

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