Cartesian harmonics and fast computation of potentials of the form $r^{-\nu}$

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Computation of potentials of the form $r^{-\nu}$ is useful in a wide range of application domains–these range from diverse areas such as computational chemistry, physics, biophysics, etc. For instance, these potentials are used very often in density functional theory. Typically, the computation of these potentials are usually cast in the framework of a N-body problem. Consequently, since the publication of the seminal papers on fast method to compute potentials of the form r^{-1} (L. Greengard, *The Rapid Evaluation of Potential Fields in Particle Systems,* MIT Press, Cambridge, MA, 1988; F. Zhao, "An O(N) algorithm for three dimensional N-body simulations," *Technical Report 995*, MIT, 1987) there have been a number of attempts to compute potentials of the form $r^{-\nu}$. While Greengard's work relies on spherical harmonic tensors, the latter relies on Taylor series expansions. All attempts to compute potentials for $r^{-\nu}$ that we have uncovered *thus far*, have used Taylor's series expansion (M. 0. Fenley, W. K. Olson, K. Chua, and A. H. Boschtisch, "Fast adaptive multipole method for computation of electrostatic energy in simulations of polyelectrolyte DNA," *J. Comp. Chem.*, **17**, 976-991, 1996; Z.-H. Duan and R. Krasny, "An adaptive treecode for computing nonbonded potential energy in classical molecular systems," *J. Comp. Chem.*, **22**, 184-195, 2001; I. Chowdhury and V. Jandhyala, "Single level multipole expansions and operators for potentials of the form $r^{-\lambda}$). This list of references is by no means complete (see numerous papers by Pardalos starting in 1996 on this very topic).

All the papers that we have encountered thus far use a Taylor's series expansion, and the analytic properties of the function, to arrive at an approximation that may be used for rapid evaluation. Our research into this rather rich field is motivated by the observation that Cartesian tensors are intimately related to spherical harmonics, in that, when properly formulated they contain the same number of independent components. Indeed, it can be shown that traceless symmetric n-th rank tensors are equivalent to spherical harmonics. Thus, using the generalized Euler's formulae, we derive the appropriate approximation to $r^{-\nu}$. Equivalent multipole expansions and their formulation to traverse up and down the tree are readily derived from this expression, and are exact. Likewise, an exact expression for the translation operator is derived using reciprocity. In the conference we will present (i) a multilevel implementation of the proposed method,(ii) proofs for the theorems that permit traversal of the tree, and (iii) convergence data.