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Real-space grid representation of momentum and kinetic energy operators for electronic structure calculations. DOMENICO NINNO, GIOVANNI CANTELE, FABIO TRANI, Università di Napoli Federico II, Dip. di Scienza Fisiche, Via Cintia, I-80126, Napoli — The development of computational methods based on real-space grids is contributing to the advances and understanding of nanoscale materials. Real-space grids methods, particularly within the pseudopotential density functional theory, have the advantage of producing highly structured matrices paving the way towards grid-based O(N) methods for both DFT total energy and molecular dynamics calculations. However, a limitation seems to be the lack of a basis set putting these approaches on a different ground with respect to standard methods. We prove that this limitation is only apparent showing that the position operator eigenkets are the natural basis set for the finite difference representation of momentum and kinetic energy operators. Some conceptual points and unpublished results related to the connection between the discrete and the continuum representations will be discussed.

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