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Orbital HP-clouds for solving Schrödinger equation in quantum mechanics. (English)

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Summary: Solving Schrödinger equation in quantum mechanics presents a challenging task in numerical methods due to the high order behavior and high dimension characteristics in the wave functions, in addition to the highly coupled nature between wave functions. This work introduces orbital and polynomial enrichment functions to the partition of unity for solution of Schrödinger equation under the framework of HP-Clouds. An intrinsic enrichment of orbital function and extrinsic enrichment of monomial functions are proposed. Due to the employment of higher order basis functions, a higher order stabilized conforming nodal integration is developed. The proposed methods are implemented using the density functional theory for solution of Schrödinger equation. Analysis of several single and multi-electron/nucleus structures demonstrates the effectiveness of the proposed method.

MSC:

81-08 Computational methods for problems pertaining to quantum theory

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Keywords:

partition of unity; HP-clouds; nodal integration; Schrödinger equation; quantum mechanics

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