THE PARTITION OF UNITY FINITE ELEMENT METHOD FOR THE SCHRÖDINGER EQUATION

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Abstract. A Schrödinger equation for the system's wavefunctions in a parallelepiped unit cell subject to Bloch-periodic boundary conditions must be solved repeatedly in quantum mechanical computations to derive the materials' properties. Recent studies have demonstrated how enriched finite element type Galerkin methods can substantially lower the number of degrees of freedom necessary to produce accurate solutions with respect to the standard plane-waves method. In particular, the flat-top partition of unity finite element method enriched with the radial eigenfunctions of the one-dimensional Schrödinger equation offers a very effective way of solving the three-dimensional Schrödinger eigenvalue problem. We investigate the theoretical properties of this approximation method, its well-posedness and stability, we prove its convergence and derive suitable bound for the h- and p-refinement in the L^2 and energy norm for both the eigenvalues and the eigenfunctions. Finally, we confirm these theoretical results by applying this method to the eigenvalue problem of the one-electron Schrödinger equation with the harmonic potential, for which the exact solution is known.

Keywords: Schrödinger eigenvalue problem, enriched partition of unity finite element method

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References

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