Multiscale Methods for Quantum Mechanics

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ABSTRACT

The first part of this work is devoted to the development of meshfree methods for solving Schrödinger equation in quantum systems. Both weak form based approaches and strong form based collocation method are proposed. We first introduce orbital and polynomial basis functions to the partition of unity for solving Schrödinger equation under the weak form framework of HP-Clouds. An intrinsic enrichment of orbital function and extrinsic enrichment of monomial functions are introduced. For general quantum systems, such as quantum dots with arbitrary size and shape, analytical orbital functions are unavailable. We introduce radial basis function as the general non polynomial basis in the approximation for quantum computation. While radial basis function exhibits exponential convergence, this approximation is suffered from the large condition numbers due to its nonlocal global approximation. The proposed reproducing kernel enriched radial basis function intends to combine the advantages of radial basis function and reproducing kernel approximation function to yield a local approximation that is more stable than that of RBF, while at the same time offers a higher rate of convergence than that of reproducing kernel approximation.

The second part of this work extends the proposed computational quantum mechanics methods to multiscale modeling of quantum-dot semiconductors and quantum-dot arrays based on asymptotic expansion. Proper coarse-fine scale coupling functions for electron energy and wave function are introduced and solved for obtaining the fine scale information of effective mass and confinement potential. Consequently, the homogenized effective mass and confinement potential are obtained using the scale coupling functions. An iterative multiscale method by introducing Reyleigh quotient that uses the solution of the first order asymptotic expansion as the initial guess is also introduce.