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RADIAL BASIS PARTITION OF UNITY GALERKIN METHOD FOR QUANTUM MECHANICS

*** J. S. Chen[1] and W. Hu[2]**

Department of Civil & Environmental Engineering University of California at Los Angeles
Los Angeles, CA90095, USA
[1]jschen@seas.ucla.edu, [2]weih@seas.ucla.edu

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ABSTRACT

Solving Schrödinger equation in quantum mechanics presents a challenging task in numerical analysis due to the nature of the highly coupled wave functions, in addition to their high order behavior and high dimension characteristics. In this work, we first introduce orbital and polynomial enrichment functions to the partition of unity for solution of Schrödinger equation. An intrinsic enrichment of orbital function and extrinsic enrichment of polynomial functions are introduced. In this first approach, orbital basis functions are reproduced everywhere in the domain of quantum system, while monomial basis functions are introduced as an additional enhancement of orbital basis functions through extrinsic enrichment to allow varying order of p-refinement. It is shown that when reproduction of orbital basis functions is enforced in the partition of unity approximation as an intrinsic enrichment, higher order extrinsic monomial enrichment is only needed in the vicinity of the nuclei.

In the second part of this work, a local radial basis function (local RBF) is introduced as the extrinsic basis functions localized by the reproducing kernel function with linear intrinsic bases. The error analysis shows that if the error of reproducing kernel is sufficiently small, the local radial basis functions maintain the exponential convergence of the global radial basis functions, while significantly improving the conditioning of the discrete system and yielding a banded matrix. The numerical results also show that radial basis functions in the second approach can be used to replace the orbital basis functions which are dependent on the electronic structure of the quantum system in the first approach. For application to quantum dot systems, a construction of the approximation functions to yield discontinuous derivative across the material interface in the proposed orbital and radial basis functions is introduced.

We examine the effectiveness of the proposed method by analyzing a spherically symmetric quantum dot composed of two materials *GaAs* and *InAs* as shown in Figure 1, where $R_1 = 300A$ is the radius of dot and $R_2 = R_1 + 100A$ is the radius of boundary

where the density of electron is assumed to be zero. Figures 2 (a) and (b) show the convergence of solutions for the first two energy levels by using the linear and quadratic FEM, the pure RKPM with linear and quadratic intrinsic bases, and the proposed local RBF constructed by using inverse Multiquadric (MQ) function localized by reproducing kernel with linear basis. The proposed local RBF achieves much better solution accuracy and convergence rate compared to other methods.

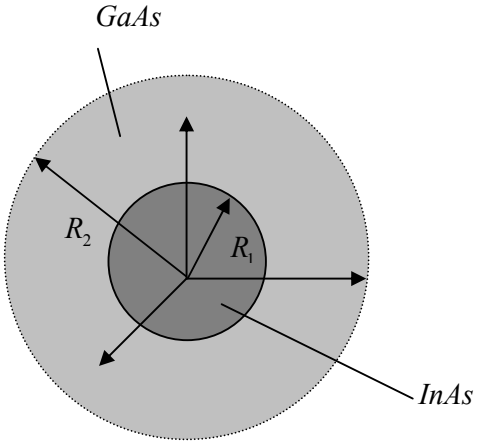
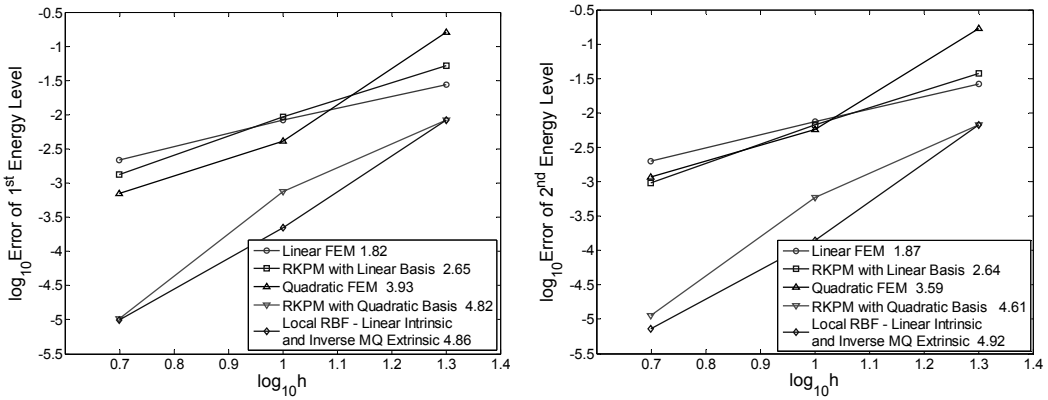


Figure 1 Model of spherical quantum dot



(a) (b)

Figure 2. Convergence of the 1st and 2nd energy levels in analysis of a spherical quantum dot

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