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SIAM Student Chapter Seminar Series

A multiscale finite element method for the Schrödinger equation with multiscale potentials

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Abstract: In recent years, an increasing attention has been paid to quantum heterostructures with tailored functionalities, such as heterojunctions and quantum metamaterials, in which quantum dynamics of electrons can be described by the Schrödinger equation with multiscale potentials. The model, however, cannot be solved by asymptotic-based approaches where an additive form of different scales in the potential term is required to construct the prescribed approximate solutions. In this paper, we propose a multiscale finite element method to solve this problem in the semiclassical regime. The localized multiscale basis functions are constructed using sparse compression of the Hamiltonian operator, and thus are "blind" to the specific form of the potential term. After an one-shot eigendecomposition, we solve the resulting system of ordinary differential equations explicitly for the time evolution. In our approach, the spatial mesh size is $H = \mathcal{O}(\epsilon)$, where ϵ is the semiclassical parameter and the time step size k is independent of ϵ. Numerical examples in one dimension with a periodic potential, a multiplicative two-scale potential, and a layered potential, and in two dimension with an additive two-scale potential and a checkboard potential are tested to demonstrate the robustness and efficiency of the proposed method. Moreover, first-order and second-order rates of convergence are observed in H^1 and L^2 norms, respectively.

Date:	20 February, 2019 (Wednesday)
Venue:	Room 219, Lady Shaw Building, The Chinese University of Hong Kong, Shatin
Time:	11:00am – 12:00noon

All are Welcome