

Schrödinger Equation Solver Based on Data-Driven Physics-Informed Generic Building Blocks

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This work investigates a physics-informed learning algorithm to solve the multi-dimensional Schrödinger equation for nanostructures based on the quantum element method (QEM) [1]. The QEM selects generic building blocks of a group of nanostructures as *elements*, each of which is trained by proper orthogonal decomposition (POD) to generate its basis functions (or POD modes). To simulate a large structure, these trained elements are then *stitched* together using the discontinuous Galerkin method. Such a multi-element approach minimizes the training effort, optimizes parallel computing efficiency, and offers cost-effective simulation and design of nanostructures.

POD trains the modes to maximize the mean square inner product with the wave function (WF) data collected from direct numerical simulation (DNS) of the Schrödinger equation. Each element is trained to account for variations of electric fields or potentials and adjacent elements. This POD process leads to the Fredholm equation [2],

$$\int_{\Omega'} \langle \psi(\vec{r}) \otimes \psi(\vec{r}') \rangle \vec{\eta}(\vec{r}') d\Omega' = \lambda \vec{\eta}(\vec{r}') \quad (1)$$

where η_j is the POD mode, ψ is the WF and λ is an eigenvalue. The eigenvalues of the POD modes indicate the amount of information captured.

After generating the POD modes, the WF can be formed via a linear combination of M modes,

$$\psi(\vec{r}) = \sum_{j=1}^M a_j \eta_j(\vec{r}) \quad (2)$$

where a_j is the weight. The weights are found via the Galerkin projection of the Schrödinger equation onto the POD modes. This projection provides physical guidance based on first principles to reach an efficient and accurate learning method.

Using the QEM for a system of N_{el} elements, the Hamiltonian equation in POD space is found,

$$\sum_{j=1}^{Mp} (T_{np,ij} + U_{\eta p,ij}) a_{p,j} + \sum_{q=1, q \neq p}^{N_{el}} \sum_{j=1}^{Mp} B_{p,q,ij} a_{p,j} + \sum_{q=1, q \neq p}^{N_{el}} \sum_{j=1}^{M_q} B_{pq,ij} a_{p,j} = E a_{p,i}, \quad (3)$$

where $T_{np,ij}$ and $U_{\eta p,ij}$ are the interior kinetic energy and potential energy matrixes for the p th element composed of M_p modes. $B_{p,pq,ij}$ is the diagonal boundary kinetic energy matrix and $B_{pq,ij}$ is the off diagonal kinetic matrix [1].

Three GaAs/InAs quantum-dot (QD) structures given in Fig. 1(a) are used to train 3 elements, 2 hexagon QD elements (see E2 and E3 in Fig. 2(a)) and one spacer element (E1 in Fig. 2(a)). Each training structure in Fig. 1(a) is subjected to 10 single component electric fields in x and y varying between $[-35, 35] kV/cm$. At each field, only WFs of the first 6 quantum states (Qs) are collected from DNS with a mesh size of 14966. Data collected from the same elements are combined to generate POD modes to account for more variations of BCs (i.e., adjacent elements).

To test the QEM method, a test electric field $\vec{E} = (25\hat{x} + 15\hat{y}) kV/cm$ was applied to the structure in Fig. 1(b). Around the 7th to 15th mode, the POD eigenvalues of all elements in Fig. 2(a) reduce from the first mode by more than 3 orders of magnitude. Figs. 2(b) and 2(c) reveal that the POD least square (LS) error is near 1% (or 2%) using just 10-15 (or 8-12) modes per element and the eigenenergies from QEM and DNS are nearly identical. $|\psi|^2$ profiles of several Qs given in Fig. 3 illustrate the excellent agreement between the QEM and DNS using only a handful of modes (DoF) per element. This study found that the QEM offers a 2-order reduction in computational time, compared to DNS.

ACKNOWLEDGMENT

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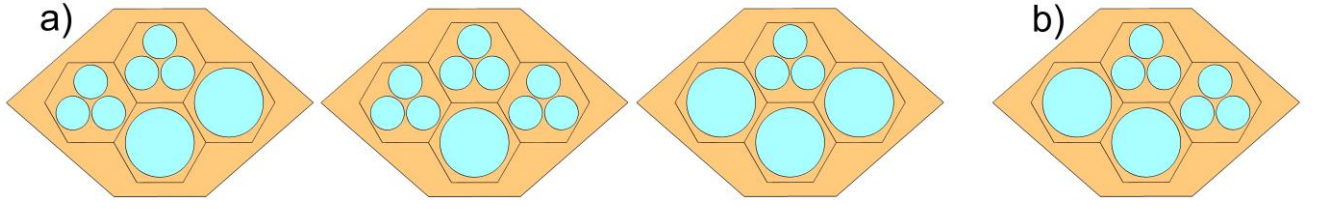


Fig. 1. (a) Three training structures used to train the 3 elements shown in Fig. 2. (b) Test structure used to verify the QEM model.

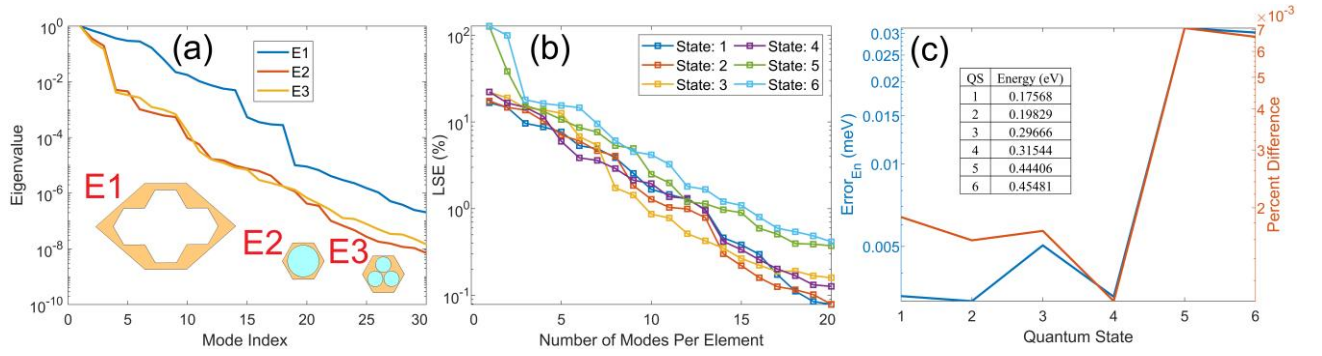


Fig. 2. (a) Eigenvalues of the three generic elements. (b) LS error for Qs 1-6. (c) Error in the QEM eigenenergy relative to DNS.

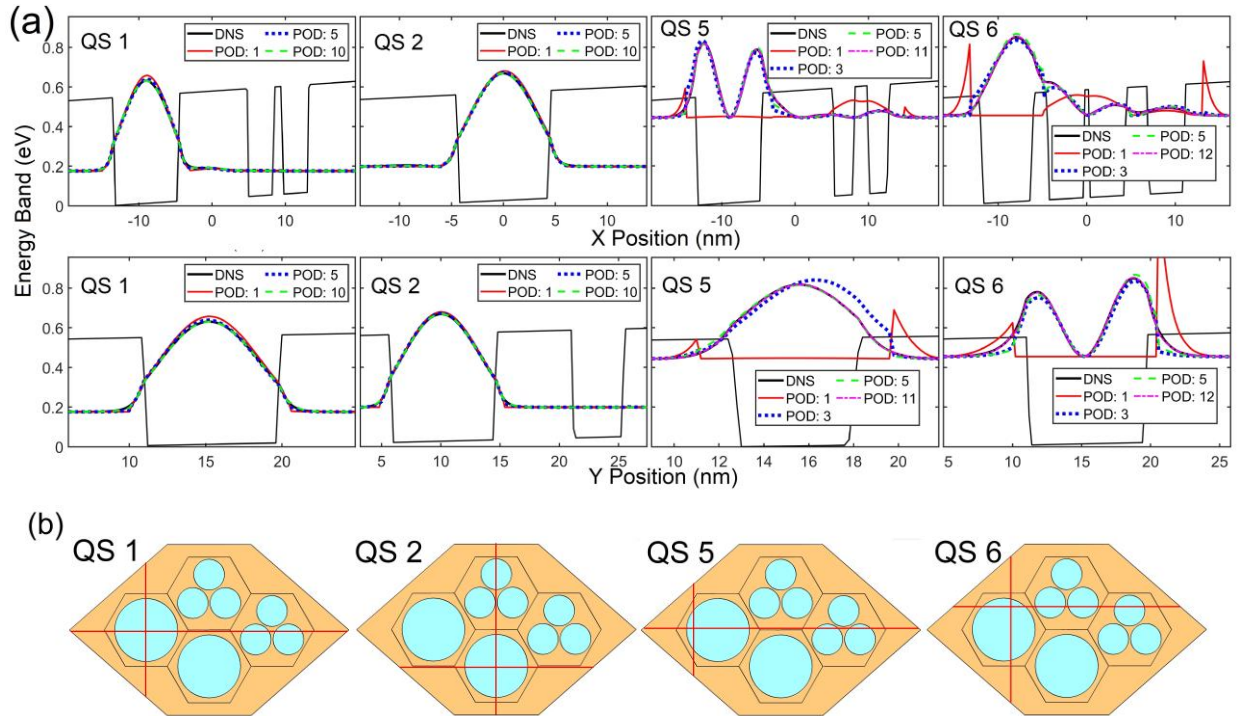


Fig. 3. (a) Profile plots in x (top row) and y (bottom row) for the $|\psi|^2$ of Qs 1, 2, 5 and 6 along the horizontal and vertical plotting paths (red lines) shown in (b). The paths were selected to show the maximum probability density in the state.