

Fast Simulations with High Accuracy for Periodic Quantum Nanostructures and Photonic Crystals Enabled by a Physics-Informed Projection Learning Methodology

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Fast solution of wave propagation in periodic structures usually relies on simplified approaches, such as analytical methods, transmission line models, scattering matrix approaches, plane wave methods, etc. For complex multi-dimensional problems, computationally intensive direct numerical simulation (DNS) is always needed. This study demonstrates a fast and accurate simulation methodology enabled by a physics-based learning methodology, derived from proper orthogonal decomposition (POD) and Galerkin projection, for periodic quantum nanostructure and photonic crystals. POD is a projection-based method that generates optimal basis functions (or POD modes) via solution data collected from DNSs. This process *trains* the POD modes to adapt parametric variations of the system and offers the best least squares (LS) fit to the solution using the smallest number of modes. This is very different from other projection approaches, e.g., Fourier, Legendre, Bessel, Airy functions, etc., that adopt assumed basis functions selected for the problem based on the solution form. After generating the optimal POD modes, Galerkin projection of the wave equation onto each of the POD modes is performed to close the model and incorporate physical principles guided by the wave equation. Such a rigorous approach offers efficient simulations with high accuracy and exhibits the extrapolation ability in cases reasonably beyond the training bounds. The POD-Galerkin methodology is applied in this study to predict band structures and wave solutions for 2D periodic quantum-dot and photonic-lattice structures. The plane-wave approach is also included in a periodic quantum-dot structure to illustrate the superior performance of the POD-Galerkin methodology. The POD-Galerkin approach offers a 2-order computing speedup for both nanostructure and optical superlattices, compared to DNS, when solving both the wave solution and band structure. If the band structure is the only concern, a 4-order improvement in computational efficiency can be achieved. Fig. 1(a) shows the optical superlattice in a demonstration, where a unit cell includes 2×2 discs with diagonally symmetrical refractive indices and the background index $n = 1$. The POD modes for this case are trained by TE mode electric field data collected from DNSs with variation of diagonally symmetrical refractive indices. The LS error of the predicted electric field wave solution from the POD-Galerkin approach, shown in Fig. 1(b) compared to DNS, is below 1% with just 8 POD modes that offer a more than 4-order reduction in the degrees of freedom, compared to DNS. In addition, an extremely accurate prediction of band structure is illustrated in Fig. 1(c) with a maximum error below 0.1% in the entire Brillouin zone.

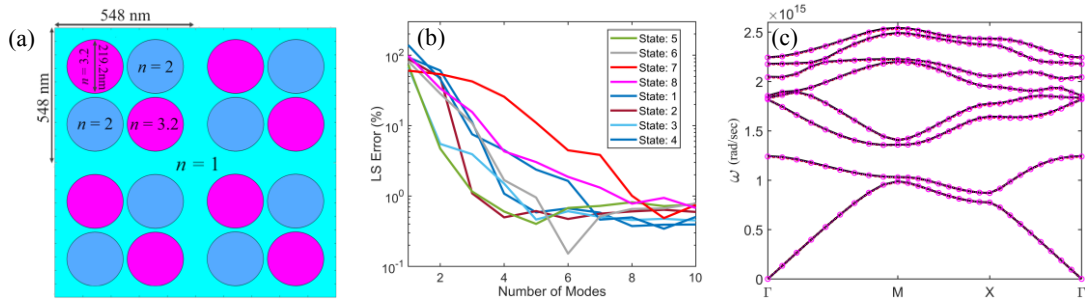


Figure 1: (a) Optical superlattice, (b) LS error of POD-Galerkin, and (c) TE mode band structure.

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