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Reduction of Order of Device Hamiltonian with Adaptive Moment Estimation

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Abstract

We have developed a method to reduce the size of device Hamiltonian for quantum transport simulation by using the adaptive moment estimation combined with auto differentiation technique. It constructs a small-size Hamiltonian which reproduces a target band structure in a narrow transport window. We implemented the method with the TensorFlow, and tested it on semiconducting nanoribbon structures. We confirmed that it correctly reproduces not only the band structures but also the transmission functions calculated by the non-equilibrium Green's function method.

1. Introduction

The non-equilibrium Green's function method (NEGF) is the one of most reliable simulation methods to analyze quantum transport characteristics of nanoscale devices [1]. Especially, the NEGF method combined with the density functional theory (DFT) is a powerful tool to simulate the device characteristics from the first principles [2]. However, it requires substantial computational resources and the efficiency of numerical algorithm is of utmost importance for simulating realistic complex device structures. We developed an equivalent model based on the basis representation [3, 4], which substantially reduces the computational burden. Here, we have proposed a method based on the adaptive momentum estimation (ADAM) [5] combined with auto differentiation technique to construct a simple model Hamiltonian with smaller size. We have implemented the method with TensorFlow [6], and tested it on nanoribbon structures.

2. Method

We construct a model Hamiltonian by minimizing the squared errors between the target and the model band structures within a narrow transport window (see Fig. 1). The minimization consists of two parts. The first part is to determine the real band structure and the second part is to determine the complex band structure, which is needed when simulating the band-to-band (or inter-band) transport characteristics. The loss functions to be minimized are then given by

$$L_{\mathrm{real}} = \frac{1}{2}\sum_{k}\sum_{i}\left(\hat{E}_i(k) - E_i(k)\right)^2 \quad , \qquad (1)$$

for the real band structure, and

$$L_{\mathrm{imag}} = \frac{1}{2}\sum_{E}\sum_{i}\left(\hat{\kappa}_i(E) - \kappa_i(E)\right)^2 \quad , \qquad (2)$$

for the complex band structure. Here $\hat{E}_i(k)$ is the target band structure (k is the wavevector and i is the band index), which should be calculated with an atomistic model such as DFT and tight-binding (TB) approximation, and $E_i(k)$ is a model band structure. Similarly, $\hat{\kappa}(E)$ is the target decay constant and $\kappa(E)$ is a model decay constant. The model Hamiltonian consists of a *on-site energy* diagonal matrix D of size $n \times n$ and a *transfer* matrix S of size $n \times n$. We have adopted ADAM with the TensorFlow to minimize L_{real} and L_{imag}. To enhance the convergence, the real and imaginary band structures were trained separately. For example, we first trained the real band structure for about several thousand loops. After that, we trained the imaginary band structure. By repeating the above procedure, we obtain the model Hamiltonian which reproduces the real and imaginary band structures.

3. Results

We have tested our method on an armchair-edge graphene nanoribbon with $N = 6$ (see Fig. 2). The target band structure is calculated with TB method whose Hamiltonian size is 12×12. The Hamiltonian size is reduced to 6×6 by the proposed method. Figure 3 shows the comparison between the target and the model band structures. We see that the model Hamiltonian correctly reproduces the target system for the lowest conduction and valence bands.

We have also tested our method for simulating the intra-band transport characteristics. We consider a zigzag-edge MoS_2 nanoribbon with $N = 5$ (see Fig. 4). The target Hamiltonian size is 59×59, which is reduced to 10×10. We see in Fig. 5(a) that the reduced Hamiltonian accurately reproduces the target system in the transport window. We applied the Eckert potential ($l = 10$ nm, $h = 0.1$ eV) [7] to the system and calculated the transmission function $T(E)$ by the NEGF method. Figure 5(b) and (c) show $T(E)$ calculated with the TB method and the proposed method, respectively. We see that the model Hamiltonian can reproduce the transmission function in the transport window.

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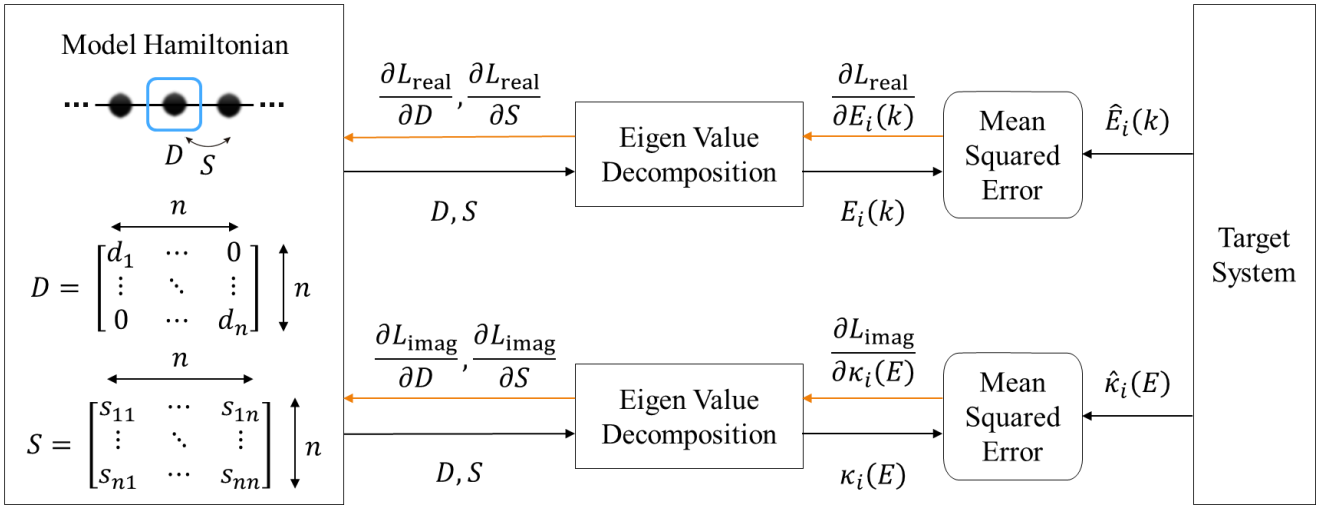
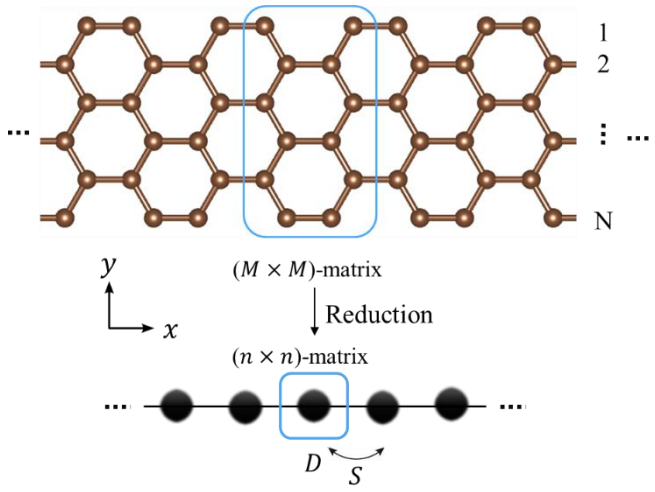


Fig. 1 Simulation flow to obtain the model Hamiltonian. The orange left-arrows represent reverse-mode differentiation.



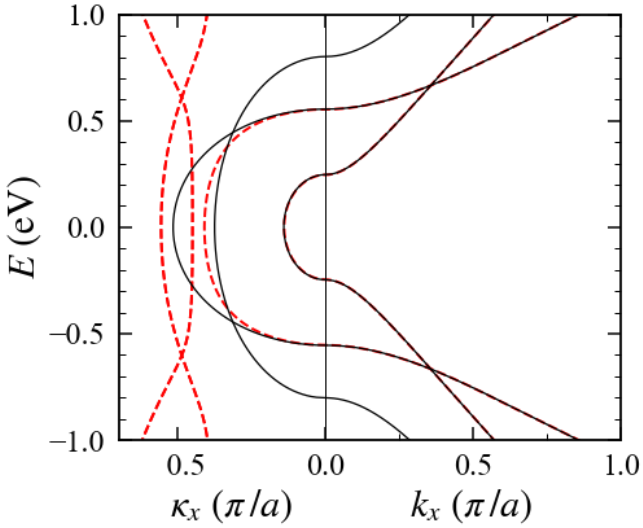
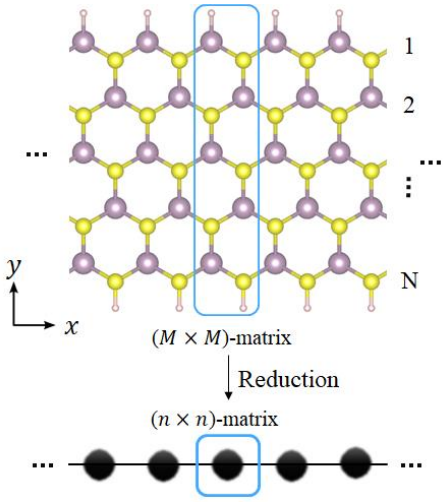


Fig. 2 [left] Armchair-edge graphene nanoribbon (top) is reduced to a model system (bottom). **Fig. 3** [right] Real and imaginary band structures calculated with TB Hamiltonian (black solid line) and the reduced Hamiltonian (red dashed line)



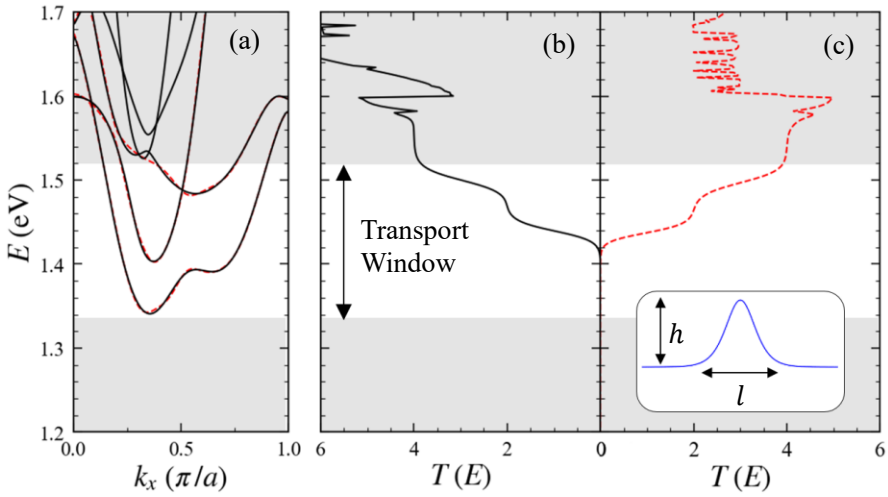


Fig. 4 [left] Zigzag-edge MoS_2 nanoribbon (top) is reduced to a model system (bottom). **Fig. 5** [right] (a) Conduction band structure calculated with TB Hamiltonian (black solid line) and the reduced Hamiltonian (red dashed line). (b) TB transmission function. (c) Transmission function calculated with the reduced Hamiltonian. Inset shows the potential profile.