Robust Mode Space Method for Heterostructure Transport Enabled by Machine Learning Approach

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INTRODUCTION

The non-equilibrium Green's function (NEGF) method combined with density functional theory (DFT) serves as a cornerstone of quantum transport simulation of nanodevices. However, its prohibitively high computational cost restricts its applicability to large-scale devices and parameter space explorations, posing a significant bottleneck for emerging nanoelectronic applications. The mode-space (MS) approach mitigates this issue by reducing the Hamiltonian dimensionality while preserving key transport characteristics [1,2]. Nevertheless, conventional MS methods struggle with non-orthogonal Hamiltonians, encountering challenges in basis selection and numerical stability leading to the need for manual efforts [2].

To address these limitations, we have developed a novel method that integrates parts of machine-learning (ML) techniques into the MS framework for homo-structure [3], which optimizes the transformation matrix U to improve computational efficiency while maintaining accuracy. Furthermore, we extend this approach to hetero-structures, where the complexity of multiple material interfaces introduces additional computational challenges.

METHOD

In this work, the transformation matrix U is initialized randomly and iteratively refined via a tailored network for the target system to accurately reproduce both the real and imaginary band structures and maximize the projectability between wavefunctions from the full and reduced Hamiltonians. By circumventing the need for manual basis selection, our approach overcomes conventional convergence issues, ensuring a stable and reliable transformation process.

For heterostructures, the device supercell is partitioned into fixed and trainable blocks as shown in Fig. 2 (a), allowing hierarchical optimization while maintaining computational efficiency. The final optimized U is then employed for NEGF-based transport simulations. The workflow of the method is shown in Fig. 1.

RESULTS AND DISCUSSION

We have applied our method to the GaSb/InAs broken-gap heterostructure depicted in Fig. 2 (a) for a tunnel FET simulation as shown in Fig. 3. The original full-Hamiltonian is obtained through DFT calculations. An optimal transformation matrix U is constructed to generate the reduced-size device Hamiltonian for transport simulations.

As shown in Fig. 2 (b), our method accurately reproduces the band structures of the target energy region. The reduced Hamiltonian for each cell has an average size of 59, approximately 9% of the original full-Hamiltonian size, as summarized in Table 1.

NEGF simulations confirm that our method faithfully reproduces key transport characteristics while significantly reducing computational cost. Fig. 4 (a) shows the band profile of the device at the ON-state, while Fig. 4 (b) presents the corresponding current spectrum demonstrating strong agreement with full-Hamiltonian results. These results demonstrate that our method accurately captures the complex tunneling properties within the hetero-junction, with high efficiency in transport simulations.

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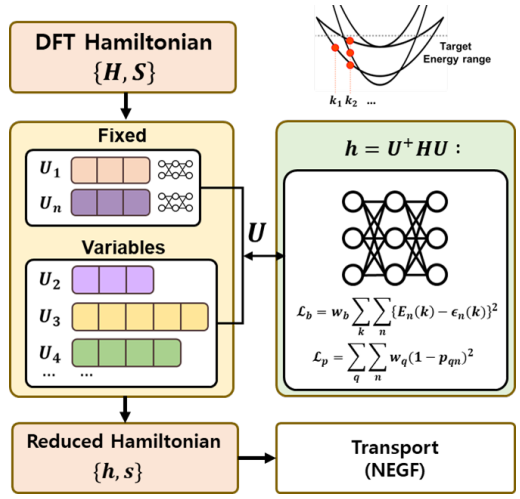

Fig. 1. Workflow of the proposed ML-assisted MS method for heterostructure transport simulations.

HAMILTONIAN REDUCTION

	L	JL2	JL1	JR1	JR2	R
Original H	616	616	616	616	616	616
Reduced H	50	50	70	70	58	58

Table 1. The sizes of the original Hamiltonian and the reduced Hamiltonian for the cells used in the transport simulation among the supercell cells in Fig. 2(a).

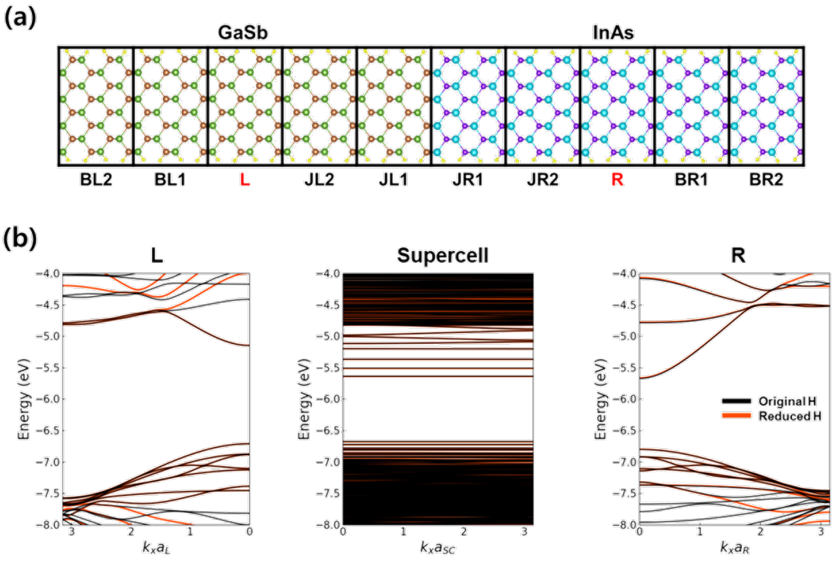

Fig. 2. (a) Atomistic configuration of 1.8 nm-thick GaSb/InAs hetero-juntion supercell with 160 Ga, 160 Sb, and 80 H atoms. The periodic boundary condition is imposed on the structure. For the heterostructure MS method, the L and R blocks are fixed, while remaining blocks are trainable. (b) Band structures of the L cell (GaSb), R cell (InAs), and 10-cell supercell (GaSb/InAs). a_L, a_R, a_{SC} represent the lateral lengths of the L cell, R cell and the supercell, respectively. The band structures are calculated at the longitudinal wave vector k_y = 0. The black and red lines represent the band structures obtained from original and reduced Hamiltonian, respectively.

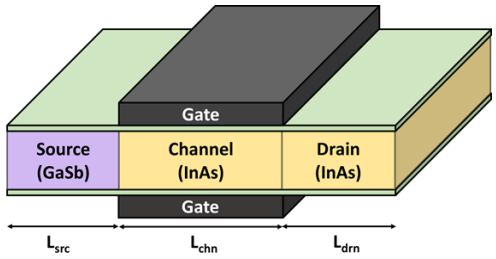

Fig. 3. Schematic of the simulated GaSb/InAs hetero-junction tunnel-FET of Fig. 2(a). The lengths of source, channel, and drain regions are 10 nm, 10 nm, and 20 nm respectively.

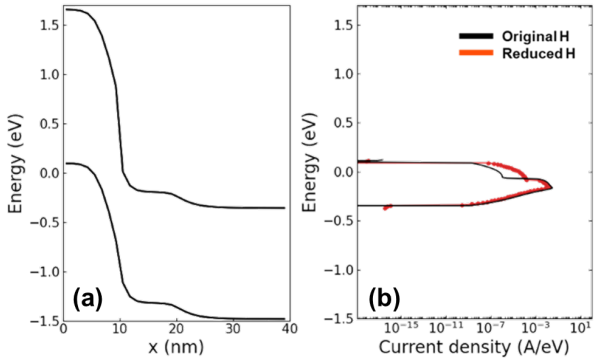

Fig. 4. (a) Band profiles and (b) comparison of the calculated current spectrum at ON-state using the original Hamiltonian (black line) and the reduced Hamiltonian (red dotted line). The applied drain bias V_{ds} is 0.5 V.