ND-map based quantum transport simulation technique application to 2D structures analysis

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INTRODUCTION

The ND-map based quantum transport simulation technique was developed few years ago to describe the charge carriers' propagation through the quantum networks. Quantum network is a union of intersecting quasi-1D quantum wires separated from the outer domain by a potential barrier. Charge carriers' propagation through such systems can be described by the scattering matrices of their elements, which, in turn, one can calculate using ND-map for Schrodinger equation.

In the current report we regard an unusual application of technique mentioned above. It is used to determine the dispersion relation in 2D periodic lattices and the effect of interlayer interaction.

This investigation is a step towards the explicit simulation of graphene electric properties on different substrates and some other recent experiments on sandwich structures.

TECHNIQUE DISCRIPTION

Neumann-to-Dirichlet map (ND-map) is a mathematical structure that relates PDE (Partial Differential Equation) solutions with Neumann boundary conditions with those with Derichlet boundary conditions. ND-map could be constructed for a wide range of linear PDE (such as Schrodinger equation) and be defined on domain of arbitrary shape. If ND-map is defined on domain then a problem with almost arbitrary (including energy-dependent) boundary condition can be solved.

The direct calculation of ND-map for Schrodinger equation requires a numeric solution of PDE on domain for every considered energy value.

We developed the technique that reduces computing resources the hundreds of times using the modification of the Green's function formalism.

APPLICATION TO 2D PERIODIC STRUCTURES

2D lattice is regarded as a periodic quantum network with the unit cell as the base element Fig. 1. The finite solutions of the Schrodinger equation with the quasi-periodic boundary conditions exist only at the points lying on dispersion curves [1]. This condition allows calculating the band structure through the unit cell ND-map Fig. 3.

Consider a sandwich of two layers Fig. 2 with the different band structures. When the interlayer interaction is taken into account, the dispersion curve intersection Fig. 4 transforms into the quasi-intersection Fig. 5.

CONCLUSION

2D lattices and 2D sandwich structures with some model potentials were treated with the ND-map based method. The obtained results are reasonable so the investigation will be preceded for real solid state systems.

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REFERENCES

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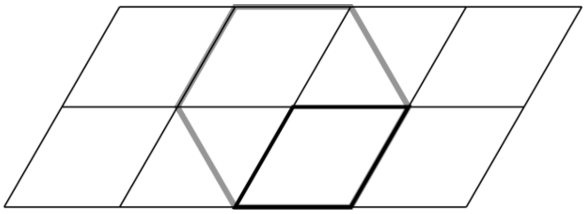

Fig. 1. 2D hexagonal lattice. Unit cell shown in bold black

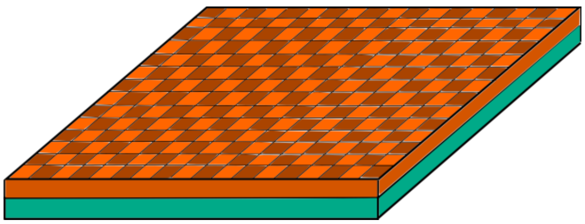

Fig. 2. Two-layer sandwich structure

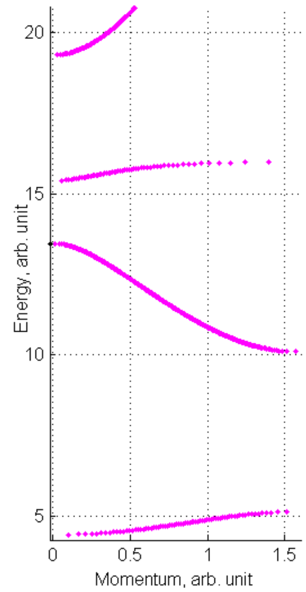

Fig. 3. Obtained 2D lattice band structure.

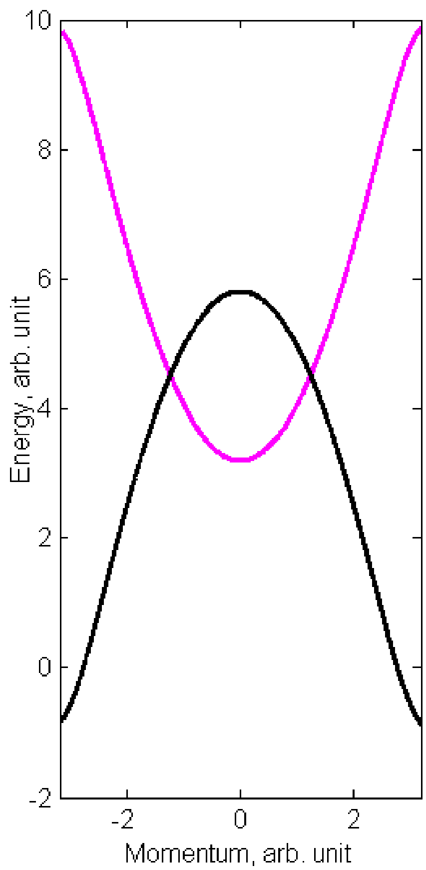

Fig. 4. Band structure of two non-interacting layers

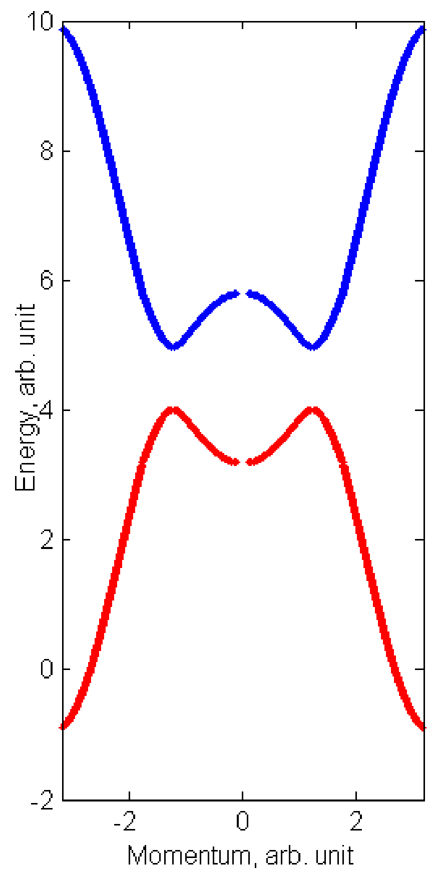

Fig. 5. Band structure of two interacting layers