Determination of bound states in a device with transmitting boundary conditions

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INTRODUCTION

Quantum transmitting boundary conditions are often imposed to determine the states in an electronic device with contacts. Transmitting boundary conditions also form the basis for most non-equilibrium Green's function (NEGF) simulations of semiconductor devices. The states in the device are calculated by considering a wavefunction with an incoming component from one mode and one contact with outgoing/decaying components in other contacts. In the wavefunction formalism the charge density is calculated by

$$n(\mathbf{r}) = \int \mathrm{d}E f_{\mathrm{L}}(E) \sum_i |\psi_{i,\mathrm{L}}(\mathbf{r};E)|^2 + f_{\mathrm{R}}(E) \sum_i |\psi_{i,\mathrm{R}}(\mathbf{r};E)|^2 \quad (1)$$

or in the non-equilibrium Green's function formalism

$$n = \int \mathrm{d}E f_{\mathrm{L}}(E) \mathrm{diag}\left(G^{\mathrm{R}}(E)\Gamma_{\mathrm{L}}(E)G^{\mathrm{A}}(E)\right) + f_{\mathrm{R}}(E) \mathrm{diag}\left(G^{\mathrm{R}}(E)\Gamma_{\mathrm{R}}(E)G^{\mathrm{A}}(E)\right). \quad (2)$$

BOUND STATES

Despite their widespread use, Eqns. (1) and (2) do not correctly describe the charge in a device if bound states are present. Moreover, even when bound states are not expected to occur in the final solutions, bound states may emerge during an iterative self-consistent process and must be properly identified and accounted for[1].

In the case of a one-dimensional potential profile, at least one bound state will be present if the potential in the device region is lower than the potential in either contact. In a two- or three-dimensional potential profile, there is no straightforward criterion for determining whether or not bound states are present.

METHOD TO DETERMINE BOUND STATES

In general the solution of the states associated with either contact are the solution of a linear system of the form

$$\left(E\mathbb{1} - H - \Sigma(E)\right) \Psi_{\mathrm{L,R}} = I_{\mathrm{L,R}} \quad (3)$$

where $\Sigma(E)$ incorporates the outgoing waves in all contacts and the right hand side $I_{\mathrm{L,R}}$ accounts for the incoming waves from left or right.

If there are bound states in the system, they will be a solution of the homogeneous system

$$\left(E\mathbb{1} - H - \Sigma(E)\right) \Psi_{\mathrm{D}} = 0. \quad (4)$$

which presents a non-linear eigenvalue problem. To solve this problem, we propose a Newton's method.

DISCUSSION

Fig. 1 shows the one-dimensional Pöschl-Teller potential which presents a textbook example of a bound state in a system with a continuous spectrum. We determine the bound states using our method. Fig. 2 and Fig. 3 show a two-dimensional canyon potential and the wavefunction of the first bound state respectively. We use an 8-band $k \cdot p$ Hamiltonian determining the CdTe/HgTe bandstructure [2] (Fig. 5) to calculate the bound states in a CdTe/HgTe/CdTe sandwich (Fig. 4). The first conduction and valence band wavefunctions are shown in Fig. 6 for two different HgTe layer thicknesses. The bound state energies are plotted as a function of HgTe layer thickness in Fig. 7 which reveals the topological insulator transition at $w \approx 6.7\,\mathrm{nm}$[3].

CONCLUSION

We have discussed the presence of bound states in a system with contacts. We have given a method to calculate the bound states and illustrated our method for the case of a one-dimensional potential, a two-dimensional potential and a one-dimensional heterostructure using the $k \cdot p$ method.

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[3] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang. *Science*, 314(5806):1757–1761, 2006.

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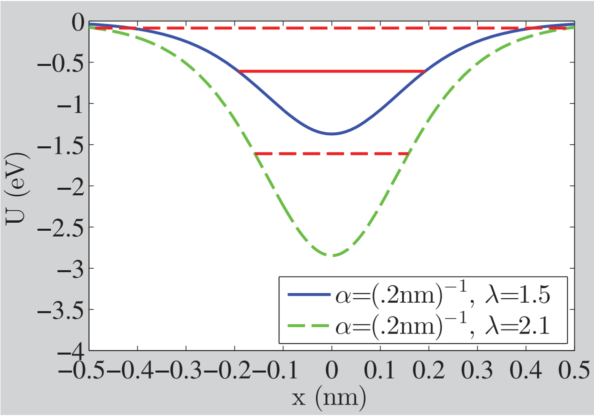

Fig. 1. Illustration of the Pöschl-Teller potential and its bound states.

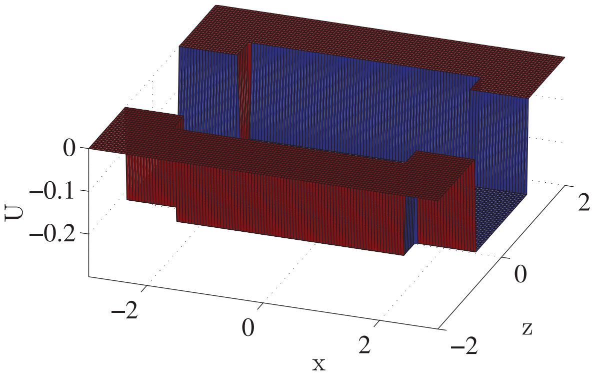

Fig. 2. Illustration of two-dimensional canyon potential harboring a bound state.

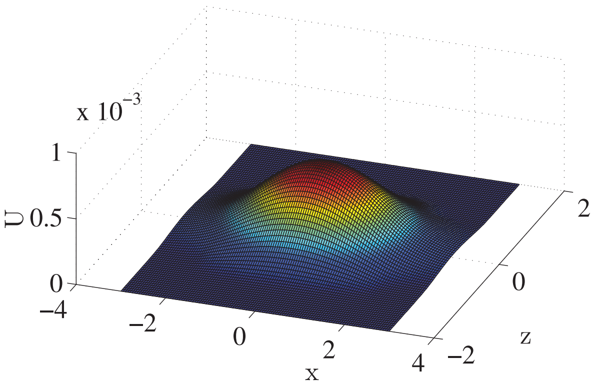

Fig. 3. Square amplitude of the first bound state in the canyon potential illustrated in Fig. 2.

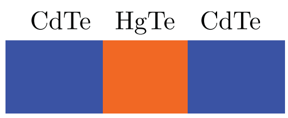

Fig. 4. Illustration of a CdTe/HgTe/CdTe sandwich.

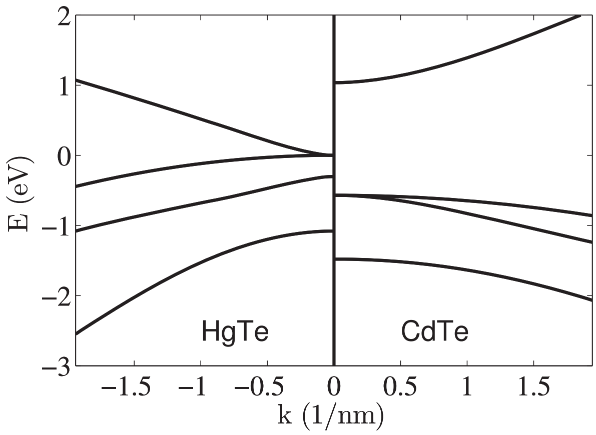

Fig. 5. Illustration of the bulk HgTe (left) and CdTe (right) bandstructure.

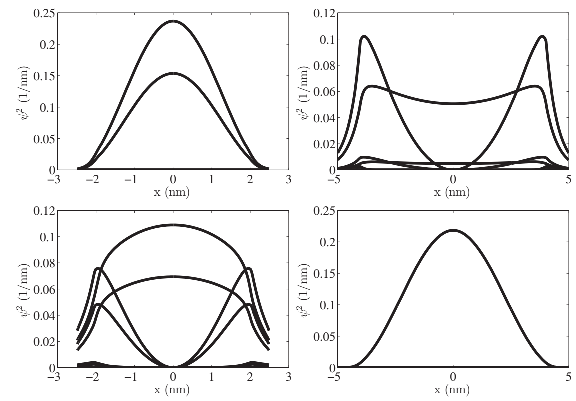

Fig. 6. $k \cdot p$ envelope functions of first conduction (top) and valence (bottom) bands for a 4 nm (left) and a 8 nm (right) sandwich.

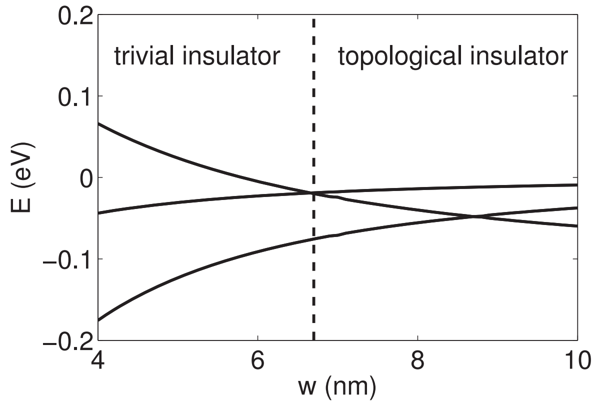

Fig. 7. Evolution of the bound state energies as a function of HgTe thickness. The transition from trivial to topological insulator can be observed at the critical thickness $w \approx 6.7\,\mathrm{nm}$.