# Band to band tunneling in heterojunctions: Semi-classical versus quantum computation

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## INTRODUCTION

Accurate and computationally efficient approaches to simulate band-to-band tunneling (BTBT) are required to optimize the performance of modern semiconductor devices. In particular, the design of Tunnel FETs (TFETs) requires very reliable BTBT simulation models since BTBT is responsible for $I_{on}$ in TFETs, whereas it only determines leakage currents in MOSFETs. Further, TCAD tools must be able to handle BTBT through heterojunctions, since for example, an appropriately designed heterojunction can boost $I_{on}$ significantly in TFETs [1].

It is known that a multiscale approach which captures the complex bandstructure within the bandgap is critical to reliably predict BTBT current through homojunctions [2], [3]. Evanescent states in heterojunctions depend on both materials forming the junction. However, semi-classical schemes to handle BTBT through heterojunctions (e.g. [4]) simply follow a region based approach, stitching together the complex bands of the two materials. The accuracy of computing BTBT current using this idea is not known. In this work, we compare this semi-classical approach against the results of an accurate quantum computation.

## PROCEDURE

Ref. [5] describes a simple two-band second-nearest neighbor tight binding model, which places a $p$-orbital on an anion and an $s$-orbital on a cation as shown in Fig. 1. We consider two direct bandgap materials A and B with a Type-II band alignment as shown in Fig. 2. Such an alignment provides a small effective bandgap $E_{g,eff}$ for tunneling and is of interest in TFET design. The electrostatic potential under applied bias is calculated using a depletion approximation. The BTBT tunneling current is written as $I = 2q/h \int T(E)dE$, where $T(E)$ is the transmission. An accurate computation of $T(E)$ is performed using the wavefunction matching method [6]. This is equivalent to the Non Equilibrium Green's Function (NEGF) method, but is simpler and more efficient. A semi-classical estimate using a WKB approximation [7] for $T(E)$ is given by

$$T(E) = -2\Big[\int_{x_1}^{0} \kappa_1(E - E_v(x))dx + \int_{0}^{x_2} \kappa_2(E - E_v(x) - \Delta E_v)dx\Big] \quad (1)$$

where $x_1, x_2$ are the classical turning points and $\kappa_1, \kappa_2$ are the imaginary bands in regions $1, 2$, $\Delta E_v = E_{v,1} - E_{v,2}$.

## RESULTS AND CONCLUSION

See Fig. 3. The semi-classical WKB approach compares very well with the quantum calculation for the case of a homojunction in a direct bandgap material [7]. On the other hand, the WKB approach significantly overestimates the current in the heterojunction. Since a quantum calculation of $T(E)$ is computationally demanding for realistic devices, our study motivates the need for better semi-classical approaches to handle BTBT through heterojunctions. Further, our procedure can be used to study this problem in other types of band alignments too.

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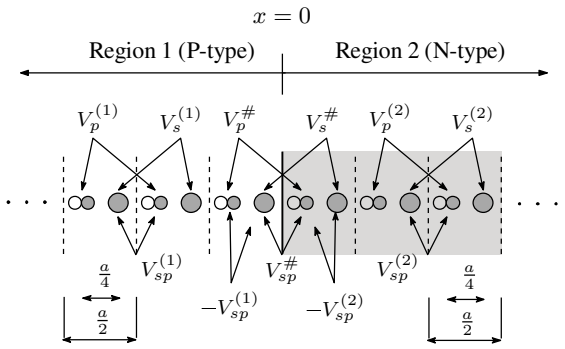


Fig. 1. A P-N junction formed using a linear chain of atoms, showing inter-atomic tight binding matrix elements [5]. $V_x^{\#} = (V_x^{(1)} + V_x^{(2)})/2$. On-site elements are $E_s^{(i)}, E_p^{(i)}$ $(i = 1, 2)$ for the $s$ and $p$ orbitals located in regions 1 and 2 respectively.

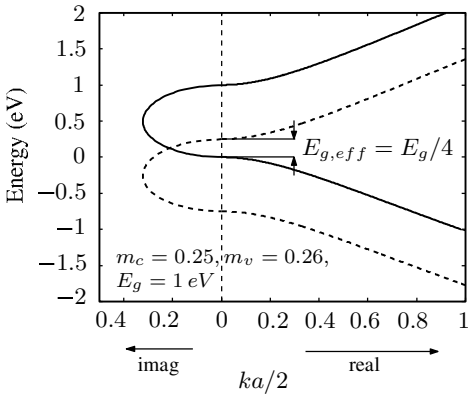


Fig. 2. Real and imaginary energy bands of Material A (solid) and Material B (dashed). These materials differ only in their electron affinities. $E_{g,eff}$ is the effective bandgap for band-to-band tunneling if Material A is P-type and B is N-type.

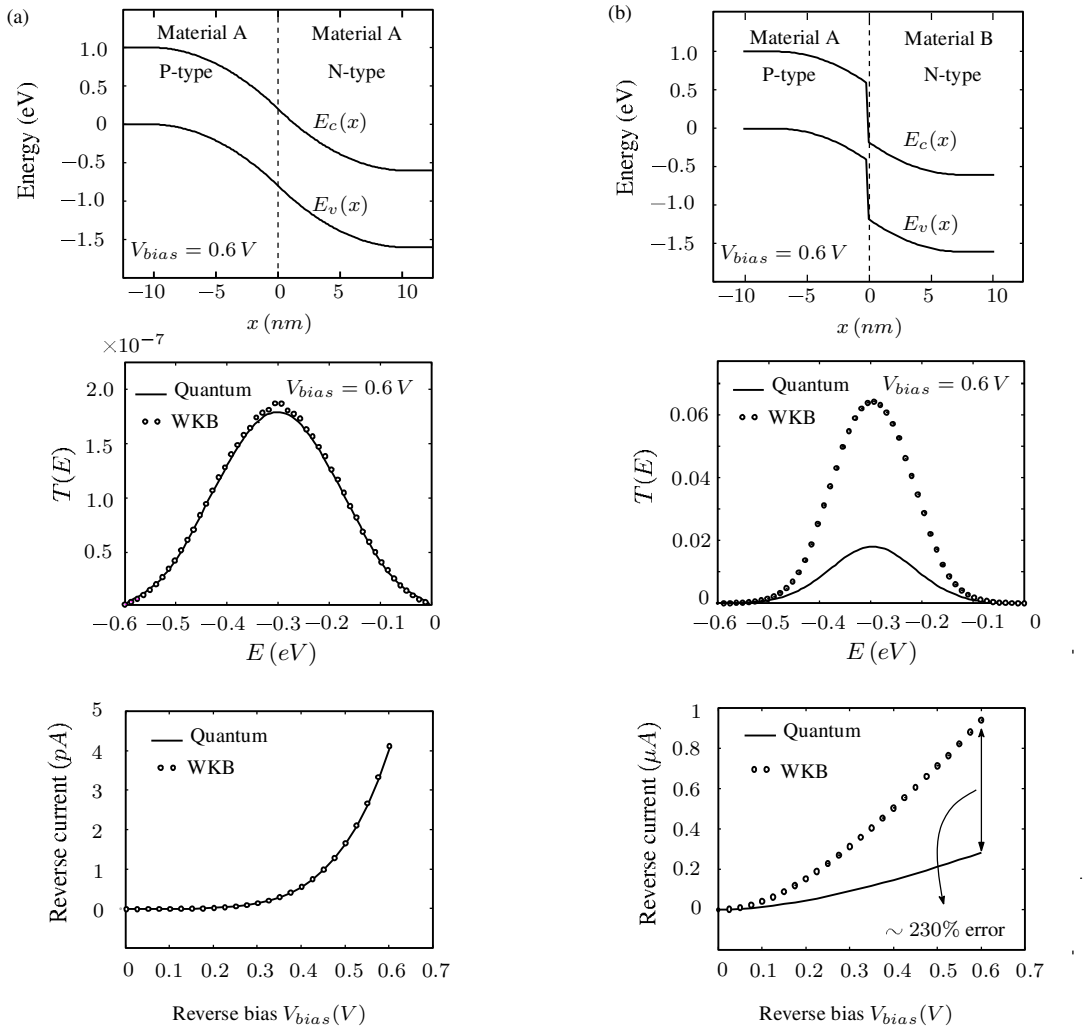


Fig. 3. Comparison of transmission $T(E)$ and current calculated using quantum and semi-classical approaches in an (a) A-A homojunction and (b) A-B heterojunction. The Fermi levels are assumed to coincide with the valence and conduction band edges on the P and N sides respectively.