

**Zeitschrift:** Helvetica Physica Acta  
**Band:** 62 (1989)  
**Heft:** 6-7

**Artikel:** Current voltage characteristics of semiconductor heterostructures : integration of sharply peaked transmissivities  
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**DOI:** <https://doi.org/10.5169/seals-116084>

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CURRENT VOLTAGE CHARACTERISTICS OF SEMICONDUCTOR HETEROSTRUCTURES —  
INTEGRATION OF SHARPLY PEAKED TRANSMISSIVITIES

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Abstract: We investigate the current through a multibarrier/quantum well heterostructure assuming conservation of energy and of the momentum parallel to the interfaces. This current is given by the Esaki integral over the transmissivity  $T(E, V_a)$ . Energies with  $T(E, 0) = 1$  correspond to the eigenvalues of the structure. For an applied voltage  $V_a$  the maxima give the resonances of the structure, whose widths are a measure for the tunneling probability through the corresponding barriers. If these probabilities are small, then the resonance lines become extremely narrow. If the precision of the computation is only a few orders of magnitude smaller, the results are very sensitive to the integration method especially near the first maximum of the  $J(V_a)$  characteristic. Here we consider an extension of the trapezoidal method, which includes an exponential grid pattern near the resonances, taking into account the strong variation of  $T(E, V_a)$ . A few examples of simple heterostructure characteristics will be discussed.

Tunneling in heterostructures [1] consisting of AlGaAs barriers (width  $b_1, b_2$ ; height  $V_1, V_2$ ) separated by a well of GaAs (width  $b_{12}$ ; height  $V_{12} = 0$ ) is the subject of intensive investigation. In the present work current-voltage characteristics derived from a simplified theory (ideal interfaces, no lateral inhomogeneities, no coherence-destroying effects such as inelastic scattering) resulting in the Esaki formula [2] are evaluated numerically. Comparison with the systematic experimental study by Guéret *et al.* will be published elsewhere [3],[4].

Consider independent quasifree electrons moving in an electric field  $V_a/L_a$  ( $L_a$  is the total length of the junction with a voltage  $V_a$  applied). Summed over the transverse  $k$ -vectors, the total current density as an integral over the longitudinal energies becomes

$$J(V_a) = \frac{em_t\theta}{2\pi\hbar^3} \int dE T(E, V_a) \ln \frac{1 + \exp(E_F - E)/\theta}{1 + \exp(E_F - E - V_a)/\theta}$$

where applied voltage  $V_a$  and temperature  $\theta = k_B T_K$  are measured in energy units (eV).  $T(E, V_a)$  is the transmissivity of the structure, i.e. the portion of electrons transmitted, which together with the reflectivity  $R$  adds up to  $T + R = 1$ .  $T$  can be found by the exact Airy-function [5] solution, whose coefficients related through four transfer matrices define  $T$ . Because of the lack of polynomial representations of Ai and Bi a plane wave approximation in subslices of width  $w$  ( $w \sim 10 \text{ \AA}$ ) is used here, assuming a constant potential in each subslice.

For our typical symmetric double barrier junctions  $b_1 = b_2 = 275 \text{ \AA}$ ,  $V_1 = V_2 = 0.12 \text{ eV}$ ,  $b_{12} = 70 \text{ \AA}$ ,  $E_F = 0.012 \text{ eV}$  and  $T_K = 4.2^\circ$ , the transmissivity exhibits resonance peaks at energies  $E_r(V_a)$ , which for small  $V_a$  are narrow and well separated. The shape is Gaussian for  $|E - E_r| \leq \Delta E_r^l$  and like  $1/(E - E_r)^2$  (Lorentzian) for  $|E - E_r| \gg \Delta E_r^l$  ( $\Delta E_r^l$  is the halfwidth of the  $r$ -th resonance) as long as the next resonance is not interfering. With increasing  $V_a$ , resonances shift towards smaller energies  $E_r(V_a) = E_{r0} - 0.5V_a + O(V_a^2)$  and increase in width according to  $\Delta E_r^l(V_a) = \Delta E_{r0}^l(1 + C_r V_a^2 + \dots)$ ; values for the above parameters are  $\Delta E_{10} = 5.2 \times 10^{-11} \text{ eV}$ , ( $C_1 = 850$ ),  $\Delta E_{20}^l = 1.7 \times 10^{-4}$ , etc. Because of the extremely small width of the first resonance, which contributes mainly to the first maximum in the  $J(V_a)$  characteristic, a special integration method has been developed. It is an extension of the trapezoidal method [6] by means of linearly distributed grid points with grid interval  $\delta E$  including an  $r$ -dependent exponential grid near resonance energies according to  $E_{r\lambda}^\pm = E_r(V_a) \pm \delta E_r p_r^\lambda$  with  $r = 1, 2, \dots$   $\lambda = 0, 1, \dots, \Lambda_r$ , where  $\Lambda_r$  is chosen such that  $\delta E_r p_r^{\Lambda_r} \cong \Delta E_r^l$ ; because of the exponential decay of the peak,  $p_r \cong 1/2$  and  $\delta E_r \cong \delta E$  give best results. The precision has been checked by halving the grid steps, which are typically  $10^{-3}$  for our example. Characteristics thus derived are reliable if the subslice width is  $w = 5 \text{ \AA}$  if the applied voltages are not too large  $|V_a| < 0.2 \text{ eV}$ .

In contrast to adaptive integration methods [6] our method avoids IF commands and is hence more appropriate for vector processor computing.

The authors acknowledge valuable discussions with A. Baratoff.

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