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Autor: Schlup, W.A. / Guéret, P.
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CURRENT VOLTAGE CHARACTERISTICS OF SEMICONDUCTOR HETEROSTRUCTURES — INTEGRATION OF SHARPLY PEAKED TRANSMISSIVITIES

W. A. Schlup and P. Guéret, IBM Research Division, Zurich Research Laboratory, CH-8803 Rüschlikon, Switzerland

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 $|E - E_r| \gg \Delta E_r^l$ (ΔE_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 $\Delta E_{10}^l = 5.2 \times 10^{-11} \text{ eV}$, ($C_1 = 850$), $\Delta E_{20}^l = 1.7 \times 10^{-4}$, 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 δE 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 Λ_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.

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