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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 ($w \sim 10$ Å) is used here, assuming a constant potential in each subslice.

For our typical symmetric double barrier junctions $b_1 = b_2 = 275$ Å, $V_1 = V_2 = 0.12$ eV, $b_{12} = 70$ Å, $E_F = 0.012$ eV and $T_K = 4.2°$, 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 $\Delta E_r^l(V_a) = \Delta E_{r0}(1 + C_r V_a{}^2 + ...)$; values for the above parameters are $\Delta E_{10} = 5.2\times10^{-11}$ eV, ($C_1 = 850$), $\Delta E_{20}^l = 1.7\times10^{-4}$, 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 $r = 1,2,...$ $\lambda = 0,1,...\Lambda_r$, 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 $w = 5$ Å if the applied voltages are not too large $|V_a| < 0.2$ 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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