обобщенная схема ее жизненного цикла, обозначены некоторые проблемы.

В дальнейших своих работах мы намерены рассмотреть и определить различия между гипотезами, предвидением и прогнозами. В частности, значительный интерес, в этом отношении, представляет анализ модели «*ПАМЯТЬ - ПРЕДСКАЗАНИЕ*» Джеффа Хокинса [5], т. к. он, с одной стороны, претендует на создание модели мозга, с другой стороны, его исследования проводятся с целью разработки систем искусственного интеллекта.

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Поступила 5.02.2009р.

УДК 72.25., 72.25.

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ELECTRON TUNNELING IN A MULTIBARRIER POTENTIAL

The electron and spin transport in nanoscopical heterostructures taking is considered taking into account features of electron spectra. It is shown efficiency of effective mass methods for an quantum-mechanical description of electron tunneling through potential barriers of the system. It is shown the description of coherent electron transport in multibarrier electron potentials.

1. Introduction

The quantum phenomena of tunneling refers to the possibility that quantum particles can traverse regions, which are from a classical point of view energetically forbidden. Tunneling is an intimate consequence of the wave properties of matter and the probabilistic interpretation of the wave function. Quantum tunneling was already considered from the early days of quantum

mechanics in connection with the problem of field ionization of atoms and the nuclear decay of alpha particles. The concept of tunneling was firstly applied in solid state physics to explain the field emission of electrons from metals into vacuum [1,2]. Single barrier tunneling has found widespread applications and one of the most prominent is the invention of the scanning tunneling microscope (STM), in which particles tunnel through a controllable vacuum barrier and which made it possible to make images on an atomic scale.

In the case of tunneling through a single barrier of height V_0, the energy-dependent transmission probability $T(E)$, which is defined as ratio of the transmitted to the incident flux, decreases exponentially with the barrier width W: $T(E) \propto \exp\left(-2W\sqrt{2m(V_0 - E)}/\hbar\right)$, where m denotes the particle mass. When a second barrier of same width is added one might intuitively suggest that, following Ohm's law, the total resistance of the structure is just doubled. This is indeed true if the region between the barriers is much larger than the de Broglie wavelength of the electrons, which in semiconductors is typically of the order of 10-100 nanometers.98 However, if the middle region is only a few nanometers in width the carrier transport remains phase-coherent and for some incident energies E_n within a small energy range of width, the particle is transmitted with a high probability, eventually up to one. This enhancement of the transmission probability is known as resonant tunneling. The physical explanation is that the resonant energies correspond to the energies of the quasibound eigenstates of the electrons, which are localized in such a state, can leak out through the barriers with a finite probability. Due to the uncertainty principle, the finite lifetime τ of the electron causes an uncertainty in the energy $\Delta E\tau \approx \hbar$, which effectively leads to the broadening of the resonance $\gamma = \Delta E \approx \hbar/\tau$. The whole process of resonant tunneling can be understood as a constructive interference between the waves leaking through the first barrier and the reflected waves of the second barrier, similar to what happens to electromagnetic waves. In a more particle-like picture corresponding to wave packets an incident electron at resonant energy tunnels through the first barrier, bounces then several times back and forth in the quantum well in a way that adds up coherently, and finally tunnels out through the second barrier.

Such double barrier structures were realized by an epitaxial growth of alternating ultrathin films of two semiconductor materials with different band gaps. Using GaAs as smaller band gap material and $Ga_{1-x}Al_xAs$ as barrier with the barrier height controlled by the molecular fraction x of Al, the conduction band profile of the layered structure exhibits sharp discontinuities at the heterointerfaces, effectively realizing a double barrier structure. The double barrier structure is usually surrounded by heavily doped layers, which provide low-resistance emitter and collector contacts. To prevent diffusion of the dopants from the high doped regions into the inner double-barrier structure usually also thin undoped buffer layers are included in experiments. By attaching ohmic contacts to the whole

structure an external bias can be applied to the resonant tunneling diode (RTD). The N-shaped current-voltage (IV) characteristic exhibits a region of negative differential resistance (NDR).

This NDR-behavior of a RTD can be qualitatively easily understood if we recognize that the electrons which are trapped between the two barriers exhibit a discrete energy spectrum whose spacing increases if the confinement gets stronger, i.e., the quantum well width becomes smaller. Let us assume, for simplicity, that the quantum well is thin enough that there is only one quasibound state in the energy range of interest. With a positive bias V_a applied to the right (collector) lead the resonant energy level is lowered relative to the energy of the incident electrons from the left (emitter) lead. In a first approximation one can assume that the voltage drops linearly from the emitter to the collector side. The electrons in the left (emitter) and right (collector) contact are considered to be always in thermal equilibrium which allows to introduce chemical potentials μ_L, μ_R for both reservoirs and to describe the electrons distribution by the Fermi-Dirac function. This means that at low temperatures incident electrons from the emitter with energies reaching from the bottom of the conduction band up to the Fermi energy are available. However, since the RTD effectively acts as an energy filter only electrons with the resonant energy E_0 can transmit to the collector side if there are unoccupied states at that energy; otherwise the electrons are blocked by the Pauli principle. By applying positive bias to the collector the resonant level passes through the emitter's Fermi energy and current starts flowing. Increasing the bias leads to higher current magnitudes. However, at a certain voltage (the peak voltage) the resonant level becomes energetically aligned with the bottom of the emitter's conduction band. Further bias pushes the resonant level E_0 below this edge, which suddenly cuts off the supply of emitter's electrons causing a sharp drop in the current and thereby leading to the phenomenon of NDR

2. Coherent tunneling

For the purpose of obtaining a more quantitative understanding of resonant tunneling and the related NDR-effect in semiconductor heterostructures we assume at first that the transport through the structure is fully phase-coherent. This assumption allows to apply a wave function treatment of the transport similar to what is done in the description of electromagnetic wave propagation in planar layers of different permittivity. We restrict our discussion primarily to electrons in a parabolic conduction band, e.g., one can think of the Γ-valley ($k = 0$) electrons in GaAs. In the case of coherent transport between two contacts the flowing current density can be obtained in general from the Landauer-Buttiker formula [1,3,4]

$$j = \frac{2e}{\hbar}\int dE\, T(E)\big(f_L(E) - f_R(E)\big),$$

where the factor 2 takes into account the spin degeneracy, e is the elementary charge, $h = 2\pi\hbar$ is Planck's constant, and $f_{L,R}(E)$ are the electrons distribution

function in the left and right reservoir, which are usually assumed to be given by Fermi-Dirac functions. The single particle transmission function $T(E)$ describes physically how likely a single electron of energy E can transmit through the structure and is more rigorously defined as the sum over all transmission probabilities $T_{n\leftarrow m}(E)$) of an electron starting in the input mode m and ending up in the output mode n of the left and right leads, respectively, which connect the reservoirs with the structure. In the specific case of planar heterostructures these lead modes are easily identified with the plain wave electron states of fixed in-plane momentum q , i.e., of a certain momentum component perpendicular to the growth direction. If we assume that the in-plane momentum is conserved during the transport, which means that there is no scattering from one lead mode to another, the transmission function can be written as

$$T(E) = \sum_{q',q} T_{q'\leftarrow q}(E) = \sum_{q',q} \delta_{q',q} T_q(E) = \sum_q T_q(E) .$$

This assumption is reasonable for elastic scatterers, which do not change the electron's momentum considerably, and as long as inelastic scattering processes are not important (which should be actually the case to allow for a phase-coherent propagation).

The transmission function $T_q(E)$ can be determined from the solution of the single-particle Schrodinger equation if the electrons can be treated as independent coherently propagating quasiparticles. This demands that the effect of electron-electron interactions is describable by an effective single-particle potential, which, by following the approach of local density functional theory, depends only on the local electron density. For simplicity we will include here only the self-consistent Hartree terms and neglect the exchange potentials or other electron-electron correlations. The influence of the periodic lattice potential of the crystal on the electrons is treated in the effective mass approximation. Under these assumptions the steady-state envelope function $\psi(r,z)$ of an single electron in the heterostructure can be determined from the Schrődinger-like equation

$$\left(\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m_l(z)} \frac{\partial}{\partial z} + \frac{\hbar^2}{2m_t} \nabla_r^2 + V_{eff}(z) \right) \psi(r,z) = E\psi(r,z) \qquad (1)$$

Here, r is the in-plane or transversal position vector and z denotes the growth direction or what we call the longitudinal direction, $m_l(z)$ is the longitudinal effective mass perpendicular to the heterointerface, $m_t(z)$ is the in-plane effective mass and E denotes the total energy. The kinetic energy operator for the longitudinal motion takes into account the z -dependence of the longitudinal effective mass and satisfies the requirement of being Hermitian. The effective potential $V_{eff}(z) = U_i(z) + U_{el}(z)$ contains the intrinsic conduction band discontinuities $U_i(z)$ and the electrostatic potential $U_{el}(z)$, which depends on the fixed ionized impurity density and the electron density profile in the structure.

Since the effective potential varies only in the longitudinal direction the in-plane motion of the electrons, which is of free electrons plane-wave type, can be separated from the growth-direction dynamics, justifying a product ansatz for the envelope function: $\psi(r,z) \propto \exp(iqr)\varphi(z)$. With this the lead input and output modes can be characterized by the plane wave states $\exp(iqr)$ Eq. (1) can be reduced to an effective one-dimensional Schrődinger equation for the growth direction motion

$$\left(\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m_l(z)} \frac{\partial}{\partial z} + V_{eff}(z) \right) \psi(r,z) = E_l \psi(r,z) \qquad (2)$$

where we introduce the longitudinal energy $E_l = E - \hbar^2 q^2 /(2m_t) = E - E_t$, which we always measure in the following from the bottom of the emitter's conduction band. From the definition of the longitudinal energy it is evident that E_t l is conserved during the transport if we assume that the total energy and the in-plane momentum q are conserved and that mt is independent of z. As we will see, these assumptions considerably simplify all further calculations, since the transmission function $T_q(E) = T(E_l)$ will only depend on the longitudinal energy, having no explicit dependence on the in-plane momenta q. According to our mean field approach for the electron-electron interaction the electrostatic potential $U_{el} = -e\phi$ can be obtained from the Poisson equation

$$\frac{\partial}{\partial z} \varepsilon(z) \frac{\partial}{\partial z} \phi(z) = \frac{1}{\varepsilon_0} \left(en(z) - \rho_{imp}(z) \right) , \qquad (3)$$

where $\varepsilon(z)$ denotes the, in general, z-dependent static dielectric constant, ε_0 is the permeability of the vacuum, $\rho_{imp}(z)$ is the fixed impurity charge density of the structure, and $n(z)$ is the electron density. The Poisson equation (3) is nonlinearly coupled to the envelope function equation (2) via the particle density $n(z)$, since the electron density profile of the structure is established by occupying the energy-dependent scattering states '(z) according to the distribution
functions of the electron reservoirs in the emitter and collector leads. Hence, the coupled Schrődinger-Poisson system has to be solved in a selfconsistent way, which can be done iteratively by alternately solving both equations and using the solution of one equation as input for the other, until convergence is reached.

In order to solve the Schrődinger equation (2) and to find the transmission function $T(E_l)$ we introduce here the transfer matrix technique (see (5-7). The basic idea of the method is to divide the z-axis into a sequence of regions where the solution can be obtained analytically. These local solutions are then composed to a global one by using the continuity conditions of the wave function between the different regions. Let us assume that we have n different layers with different effective masses m_i and constant effective potentials V_i in each layer. The solution

for each individual layer $z_{i-1} \le z \le z_i$ can then generally be written as the sum of left and right moving plane wave states

$$\varphi_i = A_i\varphi_i + B\varphi_i^* = A_i \exp(ik_i z) + B_i \exp(-ik_i z) \tag{4}$$

with $k_i = \sqrt{2m(V_0 - E)}/\hbar$ and A_i, B_i denoting the amplitudes of right and left moving waves, respectively. The continuity of the wave function and the conservation of the probability current leads to the system

$$\begin{aligned} &\varphi_i(z_i) = \varphi_{i+1}(z_i), \\ &\frac{1}{m_i}\frac{d}{dz}\varphi_i(z) = \frac{1}{m_i}\frac{d}{dz}\varphi_{i-1}(z). \end{aligned} \tag{5}$$

These relations between neighboring layers can be rewritten in matrix form,

$$U_i(z_i)\begin{pmatrix} A_i \\ B_i \end{pmatrix} = U_{i+1}(z_i)\begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix}, \quad i = 1,...,n-1 \tag{6}$$

with the matrix

$$U_i(z) = \begin{pmatrix} \varphi_i^+ & \varphi_i^- \\ (\varphi_i^+)'/m_i & (\varphi_i^-)'/m_i \end{pmatrix}, \tag{7}$$

where the prime denotes the derivative with respect to z. Starting with $i = 1$, Eq. (6) allows to express the transition amplitudes of the second layer as a function of the amplitudes of the first one, $C_2 = U_2^{-1}(z_1)U_1(z_1)C_1$, using the vector notation $C_i = (A_i, B_i)$. The matrix $M_1 = U_2^{-1}(z_1)U_1(z_1)$ is called a transfer matrix between the first and second region since it connects the corresponding amplitudes. Repeating successively this procedure for $i = 2,...,n-1$ finally allows to correlate the amplitudes of the last layer with those of the first one:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M\begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix}, \tag{8}$$

where we have introduced the composed transfer matrix,

$$M = U_n^{-1}(z_{n-1})U_{n-1}(z_{n-1})\cdot...\cdot U_2(z_2)U_2^{-1}(z_2) = \prod_{i=1,n-1} M_i \,. \tag{8'}$$

Hence, the total transfer matrix can be composed by the individual transfer matrices M_i just by using conventional matrix multiplications. The amplitudes C_1 are determined by the boundary conditions of the Schrődinger equation. For instance, if we assume only impinging electrons from the left we can set $A_1 = 1$ and $B_n = 0$. Using the relation $C_n = MC_1$ leads to $B_1 = M_{21}/M_{22}$ with M_{ij} denoting the matrix elements of M. The knowledge of the first layer amplitudes C_1 allows to successively calculate all other layer amplitudes ($C_2 = M_1C_1, C_3 = M_2C_2, ...$), constructing in this way the envelope function throughout the whole structure.

The transfer matrix connects the left and right amplitude coefficients of the structure. This representation is not unique and it is often more convenient to connect the incoming and outgoing amplitudes by the scattering matrix

$$\begin{pmatrix} B_1 \\ A_n \end{pmatrix} = S \begin{pmatrix} A_1 \\ B_n \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} A_1 \\ B_n \end{pmatrix} . \tag{9}$$

The S-matrix is a natural representation for scattering problems, since the diagonal elements are given by the reflection amplitudes r and r' for waves coming from the left and right hand side of the sample, respectively, and the off-diagonal elements are related to the wave transmission amplitudes t and t'. This physical interpretation of S_{ij} j becomes immediately evident by recognizing that the outgoing amplitudes can be always composed by reflected and transmitted parts of incoming wave amplitudes of electrons impinging from the same and opposite side, e.g., ($B_1 = S_{11}A_1 + S_{12}B_n = rA_1 + t'B_n$. By using Eqs. (8) and (9) the transfer matrix can be also expressed in terms of these wave amplitudes

$$M = \begin{pmatrix} t - r'(t')^{-1} r & r'(t')^{-1} \\ -(t')^{-1} r & (t')^{-1} \end{pmatrix} . \tag{10}$$

It should be noted that for the general case of N incoming channels the amplitudes A_1, B_1, A_n, B_n become complex vectors of length N and the transmission and reflection amplitudes are replaced by $N \times N$ matrices. The elements of the transfer matrix are not independent due to the flux conservation and other physical symmetries. For instance, for symmetric structures time reversal symmetry leads to the relation $t = (t')^T$, where the superscript T denotes transposition of the matrix. In the simple one-dimensional case, as considered here, this simplifies to $t = t'$ confirming the intuitive expectation that the transmission amplitude is the same for left and right incident electrons of equal energy, since the left-moving electron follows the time-reserved trajectory of the right moving one.

If the transmission matrix is known, the single particle transmission function $T(E_l)$ can be easily obtained as follows. Physically the transmission function is defined as the ratio of the transmitted to the incident probability flux of a particle: $T = f_{trans} / f_{inc}$. Similarly, the reflection coefficient is defined by $R = f_{refl} / f_{inc}$ with f_{refl} denoting the reflected probability flux. Conservation of the total particles flux demands that $T + R = 1$. The incident probability flux is given by the squared wave amplitude times the group velocity of the incident electron, which we assume here to impinge from the left, $f_{inc} = |A_1|^2 \hbar k_1 / m_1$, and the reflected and transmitted fluxes are accordingly determined by $f_{refl} = |B_1|^2 \hbar k_1 / m_1$ and $f_{trans} = |A_n|^2 \hbar k_1 / m_n$. With these definitions the transmission function reads as

$$T(E_l) = \frac{k_1 m_1 \mid A_n \mid^2}{k_1 m_n \mid A_1 \mid^2} .$$

By applying the corresponding boundary conditions of left incident electrons ($A_1 = 1,\ B_n = 0$) and by using the relation $C_n = MC_1$ we obtain

$$A_n = \frac{\det M}{M_{22}} A_1$$

The determinant of the transfer matrix results in $\det M = k_1 m_n / k_n m_1$, since one easily finds

$$\det[U_i(z_i)U_i^{-1}(z_{i-1})] = 1, \quad \det[U_n^{-1}(z_{n-1})U_1(z_1)] = k_1 m_n / k_n m_1$$

which can be easily verified by using the explicit expressions for M and U_i stated in Eq. (8) and (8'), respectively. With this the transmission function can finally be written as

$$T(E_l) = \frac{k_1 m_n}{k_m m_1} \frac{1}{|M_{22}|^2}. \tag{11}$$

An important point to note here is that the transmission function can also be defined as the squared current transmission amplitude $T = |\tilde{t}|^2$. The current transmission amplitude $\tilde{t}$ is related to the wave transmission amplitude t, which we have introduced in the definition of the S-matrix in Eq. (9), by $\tilde{t} = t_{L\to R} v_L / v_R$, where v_L, v_R are the left and right side group velocities. The renormalized scattering matrix based on current amplitudes, $\tilde{S}_{ij} = S_{ij}\sqrt{v_i / v_j}$, has the advantage of being unitary due to current flux conservation. With this it follows that $T(E) = (v_k / v_L)|t|^2$, which is consistent with our previous results Eq. (10) and Eq. (11) by taking into account that $\tilde{t} = \tilde{t}'$ and, hence, $t'\sqrt{v_L / v_R} = t\sqrt{v_R / v_L}$ according to time reversal symmetry

In order to investigate the basic physics of resonant tunneling we apply these general results to the special case of a double barrier structure. The typical appearance of the transmission function versus the electron's incident energy show its strongly "spiky" characteristic, the local density of states of the conduction electrons, in which the forming of quantum well states and their energetic broadening become clearly apparent. Since such a double-barrier structure consists of two single barriers in series we can calculate the total transmission matrix M by using the composition law $M = M_1 M_2$, where M_1 and M_2 are the transfer matrices of the first and second single barrier. Using the general expression given in Eq. (10) the composed transmission amplitude t results in $t = (t_1 t_2)/(1 - r_1' r_2)$, where t_i, r_i and r_i' denote the amplitudes of the single barriers $i = 1, 2$ i = 1, 2. The transmission function is given by the squared current transition amplitude

$$T(E_l) = \frac{v_R}{v_L}|t|^2 = \frac{T_1 T_2}{1 - 2\sqrt{R_1 R_2}\cos\theta + R_1 R_2} \tag{12}$$

with $T_1 = v_\omega / v_L \,|\, t_1 \,|^2$, $T_2 = v_R / v_\omega \,|\, t_2 \,|^2$ with v_ω denoting the group velocity in the well, $R_i = |\, r_i \,|^2 = |\, r_i' \,|^2$, $i = 1,2$ and θ is the phase of $r_1' + r_2$. The phase shift θ corresponds to the phase acquired by the electron when it makes one round-trip between the two barriers, which means that the electron is reflected once from each barrier before transmitting the structure. The analytical form of the transmission function T_1, T_2 for the single barriers is easily obtained from the transfer matrix technique showing an exponential dependence on the barrier width W in the limit of thick and/or high barriers $Wk_b \gg 1$, where $k_b = \sqrt{2M(V_0 - E)}/\hbar$. The expression, Eq. (12), for the composed transmission function of the double barrier structure can be further simplified if we assume, as is normally the case, that T_1, T_2, and consequently the reflection coefficients are of the order of unity, $R_1, R_2 \approx 1$:

$$T(E_l) = \frac{v_R}{v_L} |\, t \,|^2 = \frac{T_1 T_2}{\left(1 - \sqrt{R_1 R_2}\right)^2 + 2\sqrt{R_1 R_2}\,(1 - E_l \cos\theta)} \approx$$
$$\approx \frac{T_1 T_2}{[(T_1 + T_2)/2]^2 + 2[1 - E_l \cos\theta]}. \qquad (13)$$

Resonance occurs when the denominator becomes very small, which means that θ is a multiple of 2π. At resonance $T_{res} = 4T_1T_2/(T_1 + T_2)^2$, which approaches unity for the case of symmetric barriers $T_1 = T_2$. In the off-resonant case, $T \approx T_1 T_2 / 4$, indicating that the double barrier behaves as two independent barriers. Close to the resonance, $E_l = E_0$, we can further simplify Eq. (13) by performing a Taylor series expansion of the cosine function

$$1 - \cos[\theta(E_l)] \approx \frac{1}{2}\left[\theta(E_l) - 2n\pi\right]^2 \approx \frac{1}{2}\left(\left.\frac{d\theta}{dE_l}\right|_{E_0}\right)^2 (E_l - E_0)^2$$

This yields the known formula for the transmission function near the resonance,

$$T(E_l) \approx \frac{\gamma_1 \gamma_2}{(E_1 - E_0)^2 + [(\gamma_1 + \gamma_2)/2]^2}, \quad \gamma_j = \left.\frac{dE_l}{d\theta}\right|_{E_0} T_i, \qquad (14)$$

This formula was first derived in studying the decay of resonant states in nuclear problems and is often also written in the form,

$$\gamma = \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} A(E_l - E_0)$$

with the Lorentzian function

$$A(\xi) = \frac{\gamma}{\xi^2 + (\gamma/2)^2}, \quad \gamma = \gamma_1 + \gamma_2$$

This analytical expression shows that the transmission function is sharply peaked around the resonant energy E_0 and that its broadening is determined by γ, which corresponds to the full width at half maximum (FWHM) of $A(\xi)$. Physically $\gamma_1/\hbar$ and $\gamma_2/\hbar$ represents the rate at which an electron leaks out of the quantum well through barrier 1 and 2, respectively. To make this more plausible one can roughly approximate the acquired round-trip phase by $\theta \approx 2k_\omega a$, where k_ω is the longitudinal momentum of the electron in the quantum well and a is the width of the well. Hence,

$$\gamma_i/\hbar = (1/\hbar)(dE_l/d\theta)|_{E_0} \approx (1/(2\hbar))(dE_l/dk_\omega)|_{E_r}\ T_i = (v_\omega/(2a))T_i,$$

where v_ω is the group velocity of the electron in the quantum well at the resonant energy level. The attempt frequency $v_\omega/(2a)$ tells us the number of escape attempts of the electron per second through a single barrier when the electron bounces forth and back in the quantum well. Multiplying the attempt frequency by the transmission probability of the single barrier gives us the rate of successful escapes of the electron per second. Hence, the lifetime of the electron is given by the inverse of the total escape rate $\gamma/\hbar = (\gamma_1+\gamma_2)/\hbar$. Since is the FWHM of the resonant transmission peak this again leads to the general result that the energetic broadening of the quasibound state E_0 E0 is inversely proportional to the lifetime of the electron in this state. If the transmission function is known the current density can be calculated by using the Landauer-B¨uttiker formula, represented at the beginning of this section. In the case that the transmission depends only on the longitudinal energy, as considered here,

$$j = \frac{4\pi em}{(2\pi)^3\hbar^3}\int_0^\infty dE_l T(E_l)\int_0^\infty dE_t[f_L(E_l,E_t) - f_R(E_l,E_t)],$$

where we have rewritten the summation over the in-plane momentum q q in the usual integral form,

$$T(E) = \sum_q T_q = \frac{S}{(2\pi)^2}\int dq_x dq_y T(E_l)$$

with S denoting the cross sectional area of the structure, and transforming to the longitudinal and transversal energy as integration variables. Assuming Fermi-Dirac distributions in the leads

$$f_{L,R} = \left(1+\exp[(E_l+E_t-\mu_{L,R})/k_B\theta]\right)^{-1}$$

where $\mu_{L,R}$ are the chemical potentials in the left and right lead ($\mu_R = \mu_L - eV_a$ μR = μL − eVa), θ denotes the reservoir temperature to avoid confusion with the transmission T, and k_B is the Boltzmann constant, the integration over the transversal energy is easily evaluated to give the Tsu-Esaki formula [6]:

$$j = \frac{emk_B\theta}{2\pi^2\hbar^3}\int_0^\infty dE_l T(E_l)\ln\left(\frac{1+\exp[(\mu_L - E_l)/(k_B\theta)]}{1+\exp[(\mu_R - E_l)/(k_B\theta)]}\right) \tag{15}$$

The logarithmic term is the so-called supply function which determines the energy interval of interest. The range of electron energies, which can contribute to the total current, is restricted to the energy window between the left and right chemical potentials $[\mu_L \cdot \mu_R]$ plus/minus several $k_B\theta$ due to the thermal smearing of the Fermi-Dirac functions in the leads. The dominant contributions to the current integral are given by the resonant peaks of the transmission function.

If we assume that there is only one single transmission peak in the energy range of interest and that $T(E)$ is very sharply peaked around E_0 due to thick and/or high barriers we can approximate its Lorentzian form by a Dirac-Delta function by using the asymptotic limit $\delta(E_l - E_0) = \ = (1/2\pi)\lim_{\gamma\to 0} A(E_l - E_0)$. With this approximation the current density results in

$$j = \frac{e}{\hbar}\frac{\gamma_1\gamma_2}{\gamma\pi^2}k_B\theta D_0 \ln\left(\frac{1+\exp[(\mu_L - E_l)/(k_B\theta)]}{1+\exp[(\mu_R - E_l)/(k_B\theta)]}\right), \tag{16}$$

where we have introduced the constant density of states of a two-dimensional (2D) electron gas $D_0 = m/\pi\hbar^2$. In the special case of zero temperature, $\theta = 0$, this further simplifies to the expression

$$j = \frac{e}{\hbar}D_0\frac{\gamma_1\gamma_2}{\gamma\pi^2}(\mu_L - E_0(V_a)),\ 0 < E_0 < \mu, \tag{16'}$$

where the voltage dependence of the current is "hidden" in the voltage-dependent resonant energy level $E_0(V_a)$, which is shifted energetically downwards by the applied bias V_a. If we assume, in a first approximation, that the voltage is equally divided between the barriers the voltage dependence of the resonant level can be explicitly written as $E_0(V_a) = E_{00} - eV_a/2$ with $E_{00} = E_0(V_a = 0)$ denoting the resonant level position when no bias is applied. Equation (V.34) shows that the current initially increases linearly with the applied voltage, reaching its peak value

$$j_p = \frac{e}{\hbar}D_0\frac{\gamma_1\gamma_2}{\gamma}\mu_L$$

corresponding peak voltage of $eV_p = 2E_0$. At higher voltages the quasibound state becomes off-resonant causing a sudden cutoff of the current, as long as no other higher lying resonant level is pulled down into the energy window of interest

3. Sequential Tunneling

In our discussion of resonant tunneling so far we assumed that inelastic, phase-breaking scattering processes are negligible, which enables us to apply a wave function treatment of the underlying electron transport. However, if scattering is important the electrons will lose their phase memory during

propagation and the transport becomes incoherent. In this case one can use the sequential tunneling model introduced by [8]. In a sequential tunneling process electrons tunnel through the first barrier, reside some time in the quantum well where they lose coherence by phase-randomizing scattering processes and, finally, tunnel out through the second barrier by a second uncorrelated tunneling process. The regime of sequential tunneling can be characterized by the condition $\tau_{ph}\gamma \square \hbar$ saying that the lifetime $\hbar/\gamma /$ of the electrons in the quantum well is much greater than the phase breaking time τ_{ph}.

As argued by [8], NDR generally follows from the reduction of the dimensionality as the electrons tunnel from a three dimensional Fermi sea in the emitter to a 2D electron gas in the quantum well. Assuming an energy and in-plane momentum conserving tunneling process leads to the constraining condition $E_l = \hbar k^2 / 2m = E_0$, where E_0 is the energy of the resonant level in the well, measured from the bottom of the emitter conduction band. Therefore, only electrons with the fixed longitudinal momentum $k_z = k_0 = \sqrt{2mE_0}/\hbar$ can tunnel from the emitter Fermi sea into the quantum well. The maximum current is reached at the equatorial plane $k_0 = 0$. If $E_0 < 0$ no resonant tunneling from the emitter into the well is possible anymore, which leads to an abrupt drop of the current giving rise to NDR. This explanation shows that for the occurrence of NDR it does not matter if the electrons propagation is coherent or not.

To calculate the current in the sequential tunneling regime we can use a master equation approach, since the in- and out-tunneling processes become uncorrelated. For this purpose, we introduce a single particle distribution function f_α for the electron states $|\alpha>$ in the quantum well. The states $|\alpha>=|m,q>$ are characterized by the in-plane momentum q of the electrons and the subband index m, which enumerates the well quasibound states starting from the ground state $m = 0$. In real-space representation the state $|\alpha>$ reads $<r,z|\alpha>= \exp(iqr)\phi_m(z)$, where $\phi_m(z)$ is the quasibound wave function. In the leads the electrons occupy plane-wave Bloch states, shortly denoted by $|k>$. With these definitions the master equation for the quantum well distribution function reads as

$$\frac{\partial f_\alpha}{\partial t} = \sum_{j,k} \Gamma^j_{\alpha,k} f^j_k (1 - f_\alpha) - \Gamma^j_{\alpha,k} (1 - f^j_k), \qquad (17)$$

where f^j_k denotes the electron distribution function in the left and right lead ($j = 1,2 = L,R$ and $\Gamma^j_{\alpha,k}$ denotes the transition rate from state $|\alpha>$ in the lead j to the state $|\alpha>$ in the quantum well. The physical meaning of the two terms on the right hand side of Eq. (17) is easily understood. The first term is the gain term which describes the tunneling of the electrons from the leads into the quantum well

state $|\alpha>$ by taking into account the Pauli blocking factor $(1-f_\alpha)$, where as the second term describes all loss processes due to tunneling out of the state $|\alpha>$. The transition rate $\Gamma^j_{\alpha,k}$ can be calculated by using the transfer Hamiltonian approach [9,10], where it was first developed for describing single barrier tunneling and has been extensively used in the context of transport in superconducting tunnel junctions.

In the case of single barrier systems the basic idea of the method is to represent the total Hamiltonian of the system by $H = H_L + H_R + H_T$, where H_L and H_R describes the Hamiltonian of the left and right subsystem and H_T is the tunneling Hamiltonian describing the transport between the two subsystems. The main advantage of the method is that if the coupling between the two subsystems is weak, H_T can be treated as a perturbation term, which allows to use perturbative techniques developed in many-body theory. In our case of a double barrier structure the total Hamiltonian consists of three subsystems: the emitter H_L, the well H_ω, and the collector H_R Hamiltonian, which are connected by two tunneling Hamiltonians H^j_T for the left and right barrier: $H = H_L + H_R +$ $+H_\omega + H^L_T + H^R_T$. Assuming a free electron gas in the emitter and collector the corresponding Hamiltonians read $H_{L,R} = \sum_k E^{L,R}_k c^+_k c_k$ and the well Hamiltonian is given by $H_\omega = \sum_\alpha E_\alpha c^+_\alpha c_\alpha$ with c_k, c_α and c^+_k, c^+_α denoting the annihilation E_0 and creation operators of the leads and well states, respectively. The energies, $E^{L,R}_k = (\hbar k_t)^2/2m + (\hbar k_z)^2/2m + U_{L,R}$, and $E_\alpha = (\hbar q)^2/2m +$ $+U_\omega$ include the electrostatic energies of the reservoirs $U_{L,R}$ and the well U_ω. By measuring the energy from the conduction band edge of the emitter it follows that $U_L = 0$ and $U_R = -eV_\alpha$. The electrostatic potential of the well U_ω depends on the space charge density in the structure, and has to be calculated in general in a self-consistent way. The tunneling Hamiltonians are formulated in the standard form, $H^j_T = \sum_{\alpha,k} t^j_{\alpha,k} c^+_\alpha c_k + h.c.$ where $h.c.$ abbreviates the hermitian conjugate of the first term and $t^j_{\alpha,k}$ are the tunneling matrix elements. If we assume that the leads are weakly coupled to the well, the tunneling Hamiltonian can be treated as a perturbation term and the transition rates between the well and the lead states

$$\Gamma^j_{k,\alpha} = \frac{2\pi}{\hbar}\left|< k \mid H^j_t \mid \alpha >\right|^2 \delta(E_\alpha - E_k) = \frac{2\pi}{\hbar}\left|t^j_{k,\alpha}\right|^2 \delta(E_\alpha - E_k)\,.$$

By assuming that the in-plane momentum is conserved during the tunneling process this becomes $\Gamma^j_{k,\alpha} = (2\pi/\hbar)\left|t^j_m(k_z)\right|^2 \delta_{k_t,q}\delta(E_\alpha - E_k)$ with the k_z dependent

tunneling matrix element $t_m^j(k_z)$, which physically corresponds to the overlap of the lead and well wave function in the barriers and is given by [9]

$$t_m^j(k_z) = \frac{\hbar^2}{2m}\left[\psi_{k_z}^j(z)\frac{d}{dz}\phi_m^*(z) - \phi_m^*(z)\frac{d}{dz}\psi_{k_z}^j(z)\right].$$

Here, $\psi_{k_z}^j$ is the longitudinal part of the lead wave function, which is exponentially decaying in the barrier regions, the superscript * denotes complex conjugation, and the expression has to be evaluated at some point z0 inside the j th barrier-region. The total leaking rates from a certain quantum well state $|\alpha>=|m,q>$ through the left and right barriers into the leads are defined by $\gamma_2^m/\hbar = \sum_{k,k_z>0}\Gamma_{k\alpha}^2$ $\gamma_2^m/\hbar = \sum_{k,k_z>0}\Gamma_{k\alpha}^2$ which can be readily simplified to $\gamma_j^m = \sqrt{m}L/(\sqrt{2E_m^j}\hbar^2)$, $E_m^j = \hbar|k_m^j|^2/(2m) = E_m + U_\omega = U_j$ with L denoting the length of the leads. With these definitions and by exploiting the microscopic reversibility of the tunneling processes $\Gamma_{k\alpha}^j = \Gamma_{\alpha k}^j$, the master equation Eq. (17) can be written in the form

$$\frac{\partial f_\alpha}{\partial t} = \sum_j \frac{\gamma_m^j}{\hbar}[f_j(E_\alpha) - f_\alpha].$$

If we now assume, as before, that f_j are given by Fermi-Dirac distributions and that there is only one resonant level E_0 in the energy range of interest we can obtain a simple rate equation for the quantum well particle density, which is defined by $n = \sum_\alpha f_\alpha$. Summation of the master equation over all well states $\alpha = |\alpha, q>$ yields the rate equation

$$dn/dt = (\gamma_1/\hbar)n_1 + (\gamma_2/\hbar)n_2 + (\gamma/\hbar)n. \qquad (18)$$

with

$$n_j = \sum_\alpha f_j(E_\alpha) = D_0 k_B\theta \ln\left[1 + \exp[(\mu_j - E_\alpha)/(k_B\theta)]\right]$$

and $\gamma_j = \gamma_j^0$, $\gamma = \gamma_1 + \gamma_2$. This expression confirms the naive expectation that at steady state the quantum well has to establish a "compromise" between the opposing efforts of equilibrating with both leads at the same time and, hence, the particle density becomes a balanced sum of the lead particle densities weighted according to the coupling strengths to the particle reservoirs. The steady state particle density n0 follows from the condition $dn/dt = \nabla j = dj/dt = 0$ whence $n_0 = (\gamma_1 n_1 + \gamma_2 n_2)/\gamma$. Therefore, it does not matter at which z-point the current density is evaluated, and calculating the current at the first barrier yieldswhich by using Eq. (18) results in

$$j_0 = \frac{e}{\hbar}\frac{\gamma_1\gamma_2}{\gamma} k_B\theta D_0 \ln\left(\frac{1+\exp[(\mu_L - E_l)/(k_B\theta)]}{1+\exp[(\mu_R - E_l)/(k_B\theta)]}\right).$$

which is exactly the same result as we get for the coherent model in Eq. (16) in the limit of a delta-like resonant level. This limit is physically reasonable, since in order to apply the transfer Hamiltonian formalism we had to assume that the well is only very weakly coupled to the reservoirs and accordingly the electrons can stay a long time in the well before they tunnel out. A long lifetime in the well corresponds to only a very narrow energetic broadening of the quasibound states resulting in a delta-like resonance.

Thus sequential and coherent tunneling models give essentially the same values for resonant currents, although the underlying physical pictures are very different. In particular the peak current of the IV-characteristic has been shown to be insensitive to scattering. This conclusion can be justified by using a more general model that includes both a coherent and sequential part of the tunnel current (see [11]), showing that scattering processes effectively lead to an additional broadening of the resonant level. This broadening hardly influences the total current density, bearing in mind that the current is proportional to the folding integral of the transmission function with the supply function. In contrast to the peak current, the off-resonant valley current depends strongly on the presence of inelastic scattering processes.

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Поступила 12.01.2009р.