Resonant tunneling via an accumulation layer

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The electron states are investigated for a resonant-tunneling diode in which the potential well of an accumulation layer prevents electrons from tunneling coherently from source to drain at resonance energies. They may be specified as extended states, incident from the drain {anode) side and reflected back to it, or as localized discrete "quasilevel" states, almost trapped in the overall barrier system and decaying to the continuum on the anode side. The relation between these two representations is investigated. Quasilevels that are at energies not near a barrier resonance energy in general have long escape (decay) times, while a quasilevel in a certain energy range around a barrier resonance energy {forthe range of applied bias that places it there) has an escape time of the order of the Breit-Wigner response time of the resonant structure by itself. This energy range is proportional to the square root of, and in practice will be large compared with, the resonance energy width of the "stand alone" resonant structure. Resonant conduction may be expected to occur, for the corresponding bias range, by scattering transitions from the cathode source to the quasilevel followed by tunneling escape from the latter to the anode side.

I. INTRODUCTION

In electronic diode conduction by a resonant-tunneling structure, $1-3$ the normal situation has the resonant ener gy lying within the energy range of occupied states of the "electron-sea" continuum of the cathode (emitter) side. Direct coherent tunneling from the cathode source through the resonant level to the anode side is then possible. One can, however, have diode configurations where the resonant level is within the energy range of a cathode accumulation layer, especially where there is a nominally undoped spacer layer.⁴ Then electrons of the cathode continuum may reach a resonant level, and thence the anode states, via scattering processes at the site of the accumulation layer.

Figure ¹ illustrates that one can expect to have levels associated with the quantization of the accumulation layer by itself as well as levels associated with a doublebarrier (or other) resonant structure. To investigate these, it is necessary to analyze the quantum states belonging to the accumulation-layer potential and the resonant structure in combination. These quantum states

FIG. 1. Potential profile for a diode with an accumulation layer and a double barrier. The upper dotted line indicates an electron level associated with the former, away from resonance energies of the latter, and the lower dotted line a level associated with a barrier resonance.

may be considered as stationary states of the anode continuum, representing reflection on the anode side of the overall diode structure, or else as quasilevels localized within this structure but with a lifetime τ for escape into the anode continuum.

This paper presents a general analytical treatment of the electron states, in particular the latter quasilevels. It is shown that for the levels of the accumulation-layer type (corresponding to the upper dotted line in the figure) the escape time τ normally will be long. Consequently, the electrons can reach a resonance-associated level by scattering processes, before tunneling to the anode side. (Because of the lateral two-dimensional wave-vector component for electron states in a three-dimensional parallel-plane structure, it is possible for elastic disorderinduced scattering to contribute to these processes, as well as the inelastic phonon-induced scattering.) The escape time for resonance-associated quasilevels, on the other hand, will be shown to be of the same order of magnitude as the isolated ("stand alone") resonant structure's response time, $-\hbar/\Delta E$ where ΔE is the resonance half width. Where an appreciable fraction F of the norm for these electron states belongs to the accumulation-layer part of the structure, scattering rates should be comparable to those for the usual "two-dimensional electron-gas" subbands of a completely confining accumulation layer plus conventional barrier.

II. GENERAL CONSIDERATIONS

It is sufhcient here to describe the electron states in one-dimensional terms, with wave functions $\psi(x)$. For a given energy E, there are two Bloch functions $\phi_+(x)$ and $\phi(x)$, for propagation to right and to left in the anode continuum. In terms of wave vector $k(E)$, we have a velocity $v \equiv dE/d(\hbar k)$, and we write ψ in terms of coefficients (a, b) :

45 RESONANT TUNNELING VIA AN ACCUMULATION LAYER 9043

$$
\psi = v^{-1/2}(a\phi_+ + b\phi_-) \tag{2.1}
$$
 relations between the coefficients in (2.1):

with the ϕ_+ normalized in unit length. In the present case there is no transmitted wave, and so the reflection coefficient $|a/b|^2$ is equal to 1. Then the ϕ_{\pm} normalized in unit length. In the present
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with θ real for real E.

For the decaying quasilevel there is no inward wave, so we have $b=0$ and $a\neq 0$, and hence a pole of $\lambda(E)$ at a complex E value.⁵ Near a quasilevel at energy E_0 , we may assume the form

$$
\lambda(E) = -\lambda(E_0) \frac{E - E_0 - i\Delta E}{E - E_0 + i\Delta E}
$$
\n(2.3)

 $[E_0$ and ΔE real; these are not the same quantities as for Eq. (3.12) onward]. The pole is then at $E = E_0 - i\Delta E$. Since $|\psi|^2$ varies with time t as $\exp[i(E^* - E)t/\hbar]$, the decay time is

$$
\tau = \hbar / 2\Delta E \tag{2.4}
$$

The formal reflection delay time is $t_r = \hbar d(\text{arg}\lambda) / dE$ = $\hbar d\theta/dE$ for real E, and so from (2.3) and (2.4) we have $t_r(E)=4\tau\Lambda$, (2.5)

$$
t(F) = 4\pi\Lambda \tag{2.5}
$$

where

$$
\Lambda(E) = 1 / \{1 + [(E - E_0) / \Delta E]^2\}
$$
 (2.6)

is the standard Lorentzian, with half width ΔE .

Finally, we need to investigate the normalization, within the overall reflecting structure, for the extended within the overall fenecting structure, for the extended
(real E) states. Let $\mathcal{N} \equiv \int |\psi|^2 dx$ be the norm, with the integral extending over this (accumulation layer plus resonant barrier) structure. For an incident wave normalized in unit length $(|a| = v^{1/2})$ let $\mathcal{N} = l$, defining the "normalization length" $l(E)$. Then for the state normalized over a macroscopic length L (the anode space) we will have $\mathcal{N} = l / 2L$. The density of states with that normalization is $\rho(E) = L / \pi \hbar v$. To define a single quasibound state in this situation we should have $\int N \rho dE = 1$, and therefore $\int (l/v) dE = 2\pi \hbar$. This is satisfied by

$$
l/v = 4\tau \Lambda(E) = t_r \tag{2.7}
$$

Thus l/v , which is usually called the "dwell time" in the context of resonant transmission, may be equated to the formal reflection delay time. That is the intuitive result, although in resonance conditions the significance of a wave-packet transit time is questionable. The result (2.7) is analogous to what has been obtained for resonant transmission.

III. ELECTRON STATES OF THE SYSTEM

The method of this paper is to partition the reflecting structure into its two components, and combine them in terms of the parameters characterizing the resonant part. For the accumulation-layer part, it is expedient to use the representation (2.1) in some WKB sense (see below). For the resonant barrier part, its "stand alone" properties are given by the 2×2 transmission matrix $M(E)$ of the linear

$$
a_R = Pa_L + Ub_L ,
$$

\n
$$
b_R = Va_L + Qb_L ,
$$

\n(3.1)

connecting the accumulation-layer side of the resonant barrier ($L=$ left) to its anode side ($R =$ right). This matrix satisfies

$$
det M \equiv PQ - UV = 1 \tag{3.2}
$$

for all E, and $Q = P^*$ and $V = U^*$ for real E. The standalone transmission probability for this component of the barrier system is

$$
T(E) = 1/PQ \tag{3.3}
$$

and, by (3.2), the refiection probability is then

$$
R = 1 - T = UV/PQ \tag{3.4}
$$

The extended states are given by real E , with The extended states are given by
 $|a_L/b_L| = |a_R/b_R| = 1$. Accordingly we set

$$
a_L/b_L = \exp[2i\chi(E)] \tag{3.5}
$$

(where the phase χ will, when convenient, be taken to be given by $\int k \, dx$ on the L side) and

$$
U/P = R^{1/2} \exp(i\eta) \tag{3.6}
$$

(2.6) Then

$$
|a_R/a_L|^2 = (1/T)|1 + R^{1/2} \exp(-i\Omega)|^2
$$

= (1/T)[(1-R^{1/2})^2 + 4R^{1/2} \cos^2\Omega/2], (3.7)

where $\Omega \equiv 2\chi - \eta$.

At E values far from a barrier resonance, we will generally have $T \ll 1$ and varying slowly with E. Then, by (3.7), to a sufficient approximation $|a_L/a_R|^2$ versus E has (3.7), to a sumerist approximation $|u_L/u_R|$ versus E has
a sharp maximum equal to $T/(1-R^{1/2})^2=4/T$ at a value $E = E_0$ satisfying $\Omega(E) = (2n + 1)\pi$ for n an integer, and a Lorentzian E dependence (2.6) with

$$
\Delta E = (T/2)|dE/d\Omega| \tag{3.8}
$$

(these quantities being evaluated at $E = E_0$). A physical interpretation of (3.8) comes from taking the path contribution to $d\chi/dE$ as $(d/dE)\int k dx = (1/\hbar)\int (1/v)dx$ and hence, on adding a reflection delay time from the η term (the reflection phase being $\pi-\eta$), identifying $\hbar|d\Omega/dE|$ as t_p , the "path time" for an itinerant electron to traverse the accumulation layer once in each direction without escaping. Then from (2.4) and (3.8)

$$
\tau = t_p / T \tag{3.9}
$$

in agreement with the heuristic expectation that $1/\tau$ should be equal to T times the "attempt frequency" $1/t_p$. The factor T (which away from a barrier resonance will be $\approx T_L T_R$, where T_L and T_R are the separate transmission probabilities of the pair of barriers, in the case of a double barrier) should make the escape time long compared to $t_n \approx \hbar / E$. For the normalization length, we should evidently multiply the maximum value, $4/T$, of

 $|a_L/a_R|^2$ by $t_p v$ [that is, $t_p v/2$ for each of $|a_L|^2$ and $|b_L|^2$ —and so without the ζ factor of (3.22) which applies in that case], obtaining $l=4\tau v$ at resonance, in agreement with (2.7).

We may also analyze the quasilevels in terms of (3.1), still for E far from a barrier resonance. The condition for $b_R = 0$ is

$$
a_L/b_L = -Q/V \tag{3.10}
$$

Together with (3.5) this gives

$$
R^{1/2} + \exp(-i\Omega) = 0 \tag{3.11}
$$

Writing $\Omega = \Omega' + i \Omega''$ (real and imaginary parts), we have that (3.11) is satisfied by $\Omega' = (2n+1)\pi$ and, to sufficient approximation for $T \ll 1$, by $\Omega'' = -T/2$ (neglecting here the variation of R due to Ω''). Taking Ω'' $=E''(d\Omega/dE)$, this result agrees with the value of τ according to (2.4) and (3.8) .

To analyze a quasilevel associated with a barrier resonance, we expand the right-hand side of (3.10) about the
"stand alone" resonance energy, in terms of $z = (E - (E - E))$ "stand alone" resonance energy, in terms of $z \equiv (E - E_0)/\Delta E$, where E_0 and ΔE will hereafter refer to the resonant barrier system —such that its "stand alone" transmission probability is $T(E) = T_0 \Lambda(E)$ where Λ is given by (2.6) and the maximum $T_0 = T(E_0)$ is given by (3.14). (This ΔE could be ~ 1 meV.) It can be shown⁷ that, near this E_0 ,

$$
Q = Q_0(1 - iz), \quad V = V_0(1 - iz \sigma R_0^{-1/2}), \quad (3.12)
$$

where $Q_0 \equiv Q(E_0)$, etc., where $R_0 = 1 - T_0$ is the value of R at $E = E_0$, and where, in terms of the leftward and rightward decay currents I_L , I_R for the quasilevel of the "stand alone" resonant system, $\sigma = +1$ if $I_R > I_L$ and $=-1$ if $I_L > I_R$. (We expect the former case, because of the applied bias.) We make use of the formulas⁷

$$
1 + \sigma R_0^{1/2} = 2I_R / (I_L + I_R) \equiv 2\gamma_R ,
$$

$$
1 - \sigma R_0^{1/2} = 2I_L / (I_L + I_R) \equiv 2\gamma_L ,
$$
 (3.13)

and

$$
T_0 = 4I_L I_R / (I_L + I_R)^2 = 4\gamma_L \gamma_R \tag{3.14}
$$

Since $Q_0/V_0=R_0^{-1/2}$ exp(i η_0), Eqs. (3.5) and (3.10) with (3.12) give

$$
\frac{1 - iz}{R_0^{1/2} - i\sigma z} + \exp(i\Omega) = 0 ,
$$
 (3.15)

where here $\Omega = 2\chi(E) - \eta_0$. An appropriate approximation in (3.15) is $\Omega = \Omega_0 + 2\alpha z$, where $\Omega_0 \equiv \Omega(E_0)$ and

$$
\alpha = \frac{\Delta E}{2} \frac{d\Omega}{dE} = \Delta E \frac{d\chi}{dE} \tag{3.16}
$$

It is applicable since we will have $\alpha \ll 1$. The resulting equation

$$
\frac{1-iz}{R_0^{1/2}-i\sigma z} = -\exp[i(\Omega_0+2\alpha z)]
$$
\n(3.17)

for complex $z = x + iy$ in terms of Ω_0 has a solution with $x=0$ when $exp(i\Omega_0) = \sigma$. For $\sigma = +1$, it is given by $\Omega_0 = 2n\pi$, and x sweeps through zero (E' sweeps through

 E_0) as Ω_0 – 2n π passes through zero. This is the range of the long-lived resonant quasilevels. They are thus "antilevels" relative to the levels away from this resonance energy range, which are at $\Omega_0 = (2n + 1)\pi$. It is useful to treat y as a function of x, rather than of Ω_0 , as independent variable. Taking the modulus of each side of (3.17), we have

$$
(1+y)^2 - (\sigma R_0^{1/2} + y)^2 \exp(-4\alpha y)
$$

= $-x^2[1-\exp(-4\alpha y)].$ (3.18)

Since $\alpha \ll 1$, an appropriate approximation is to drop the $exp(-4\alpha y)$ on the left and replace the second factor on the right by $4\alpha y$. Then, to sufficient approximation,

$$
y = -\frac{\gamma_L \gamma_R}{\gamma_L + \alpha x^2} \tag{3.19}
$$

Thus, when x^2 is small compared to γ_L / α the decay rate is γ_R times the "stand alone" resonant-state value $2\Delta E/\hbar$, and as x^2 increases the rate falls off when $(E'-E_0)^2 \approx \gamma_L \Delta E/(d\chi/dE).$

Scattering to this quasilevel will depend on the norm fraction

$$
F = \mathcal{N}_{\text{acc}} / \mathcal{N} \tag{3.20}
$$

where \mathcal{N}_{acc} is the accumulation-layer part of the norm $\mathcal{N} = \int |\psi|^2 dx$ for the overall barrier structure. A decay rate of $1/\tau$ corresponds to

$$
|a_R|^2 = \mathcal{N}/\tau \tag{3.21}
$$

for the wave function on the anode side. This compares For the wave function on the anode side. This compare
with $\mathcal{N}_{\text{acc}} = \int_{\text{acc}} |\psi|^2 dx = \xi (|a_L|^2 + |b_L|^2) \int_{\text{acc}} (1/v) dx$ where ξ is a factor from the degree of nonorthogonality of the ϕ_+ and ϕ_- terms of ψ in the integral \mathcal{N}_{acc} . The ξ factor depends on the potential profile and $v(E, x)$, and evidently cannot be evaluated in general terms. However, consideration of the "square-well" case indicates that it oscillates about ¹ over a limited range, and so does not change the order of magnitude of F . We have

$$
\mathcal{N}_{\text{acc}} = \xi(|a_L|^2 + |b_L|^2)\hbar \, d\chi/dE \tag{3.22}
$$

and therefore

$$
F = 4\xi\alpha(-y)\frac{|a_L|^2 + |b_L|^2}{2|a_R|^2} \tag{3.23}
$$

On substituting $b_R = 0$ in (3.1) and making use of (3.2), we obtain $a_L / a_R = Q$ and $b_L / a_R = -V$. The final factor of (3.23) is therefore equal to $(|\mathcal{Q}|^2+|V|^2)/2$. With use of the approximations leading to (3.19), this factor becomes $[(1+y)^2+(1+2\alpha y)x^2]/T_0$. The 2ay will be small compared with 1, and may be dropped. Then, on substituting from (3.14) and (3.19), we have

$$
F \simeq \xi \alpha \frac{(1+y)^2 + x^2}{\gamma_L + \alpha x^2} \ . \tag{3.24}
$$

For $x^2 \lesssim 1$, this will be small, because of the initial factor α . For $x^2 \gg 1$, it becomes $\xi \alpha x^2/(\gamma_L + \alpha x^2)$. Thus F increases to ξ when $\alpha x^2/\gamma_L$ becomes large. This result seems somewhat anomalous, because apparently one could have $F > 1$. However, for the "square-well" case one finds that $\xi - 1$ has the same sign as η_0 , and analysis of the double-barrier structure shows that $\eta_0 < 0$ when E is less than half the height of the barrier on the L side. In this case, at least, we can expect $\xi < 1$. There remains a question of how far results here are dependent on the assumption, at various points, of a WKB form for $\psi(x)$ in an accumulation layer (rather than, for example, Airy functions). An alternative treatment in terms of a model Hamiltonian $⁸$ with coupling elements at the two boun-</sup> daries of the resonant structure, applied to this system so as to couple component states in the two regions, should give overall barrier states with $F \lesssim 1$, which then become quasilevels decaying into the anode continuum.

Kinetic analyses of the current through this system of levels, in its three-dimensiona1 context, are algebraically complicated. We may examine the effect of variation of τ and F, for a single quasilevel near E_0 , by a simple model in which it is assumed that the levels from which this level is filled by scattering processes remain full. Then the current passing through the quasilevel is proportional to

$$
I = (1 - f)F / (\xi \tau_1) = fG / \tau_2 , \qquad (3.25)
$$

where f is the occupation probability of the quasilevel, $1/\tau_1$ is the rate of scattering into it when $F=\xi$, the maximum rate of escape by tunneling out of it (i.e., for $x=0$) is $1/\tau_2$, and G is the factor given by (3.19) as $-y/\gamma_R$. Eliminating f from (3.25), we have

$$
\frac{1}{I} = \frac{\xi \tau_1}{F} + \frac{\tau_2}{G} \tag{3.26}
$$

On substituting in (3.26) for F and G from (3.19) and (3.24), to a sufficient approximation $I(x)$ has a maximum of $1/(\tau_1^{1/2} + \tau_2^{1/2})^2$ at $\alpha x^2 / \gamma_L = (\tau_1/\tau_2)^{1/2}$.

If we set $\Omega_0 = 2n\pi + \omega$ (so that ω varies with x), then the corresponding bias increment is presumably given by E_1/e where

$$
E_1 \simeq (dE/d\Omega)\omega = (\Delta E/2\alpha)\omega \ . \tag{3.27}
$$

From (3.17), in the conditions of interest we will have $\omega \approx -2\alpha x$ for a quasilevel. Hence $E_1 \approx -x\Delta E$. The range of interest for $x \Delta E$, and therefore for E_1 , is $\sim \Delta E \alpha^{-1/2}$. Since the conventional level spacing, for the $\sim \Delta E \alpha$. Since the conventional level spacing, for the
accumulation layer, is $\delta E = \pi dE/d\Omega$, this range is
 $\sim (\Delta E \delta E)^{1/2}$, the geometric mean.⁹ The effective energy width for resonance current is thus in practice large compared with ΔE , an unexpected result.

IV. DISCUSSION

The foregoing general treatment has shown that (a) the quasilevels at energies far from the barrier resonance energy, associated with the accumulation layer, in general have relatively long decay times; and (b) quasilevels in a relatively small range of energies near a barrier resonance energy have decay times comparable with the characteristic response time $\hbar/2\Delta E$ of the resonant barrier structure, and for a substantial part of this range most of their norm $\int |\psi|^2 dx$ is within the accumulation layer. Hence we expect a diode current due to scattering into these resonance-associated levels from the cathode side and out of them to the anode side, for the corresponding range of the external bias.

One would expect a detailed treatment of the kinetics to be most successful by a Monte Carlo method (adapted to allow for degeneracy in the occupation of the states). However, this presumes prior numerical calculation of wave functions, and thereby calculation of the strengths of the scattering processes for localized and continuum states. ¹⁰ One would seek to compute wave functions for
the extended, stationary (real E) states, rather than for
the decaying quasilevels. The normalization length $l(E)$
would be calculated. Its maximum, $l_0 \equiv l(E_0)$, the extended, stationary (real E) states, rather than for the decaying quasilevels. The normalization length $l(E)$ give the location of E_0 . A Lorentzian variation of $l(E)$ about E_0 would give a half width ΔE and hence a value of $\tau = \hbar/2\Delta E$, and should verify the relationship l_0 $=2\hbar v/\Delta E$. As is elucidated above, one will need a delicate precision as a function of E_0 , for many values in a small E range. Techniques for such computations have
been demonstrated.¹¹ been demonstrated.¹¹

- ${}^{1}R$. Tsu and L. Esaki, Appl. Phys. Lett. 22, 562 (1973).
- ²L. L. Chang, L. Esaki, and R. Tsu, Appl. Phys. Lett. 24, 593 (1974).
- ³T. C. L. G. Sollner et al., Appl. Phys. Lett. 43, 588 (1983).
- 4J. S. Wu et al., J. Appl. Phys. 69, 1122 (1991).
- ⁵Such a formulation was originally used in discussing α decay of atomic nuclei, by G. Gamow, Z. Phys. 53, 601 (1929).
- 6L. Gu and B.Y. Gu, Solid State Commun. 72, 1215 (1989).
- 7P.J. Price, Phys. Rev. B38, 1994 (1988).
- ⁸N. S. Wingreen, K. W. Jacobsen, and J. W. Wilkins, Phys. Rev. B40, 11 834 (1989).
- ⁹Essentially this result has been obtained by F. W. Sheard and G. A. Toombs (unpublished), independently by use of a different model.
- L. Liang and C. S. Lent, J. Appl. Phys. 68, 1741 (1990).
- ¹¹C. Jacoboni and P. J. Price, Solid State Commun. 75, 193 (1990).