INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE CENTRATOM TRIESTE

SMR.459 - 26

SPRING COLLEGE IN CONDENSED MATTER ON:
"PHYSICS OF LOW-DIMENSIONAL STRUCTURES"

(23 APRIL - 15 JUNE 1990)

"TUNNELLING"

(plus Background Material)

G.D. GARCIA-CALDERON
Universidad Nacional Autonoma de Mexico
Instituto de Fisica
Apdo. Post. 20-364
Delegacion Alvaro Obregon
Mexico City 01000
Mexico

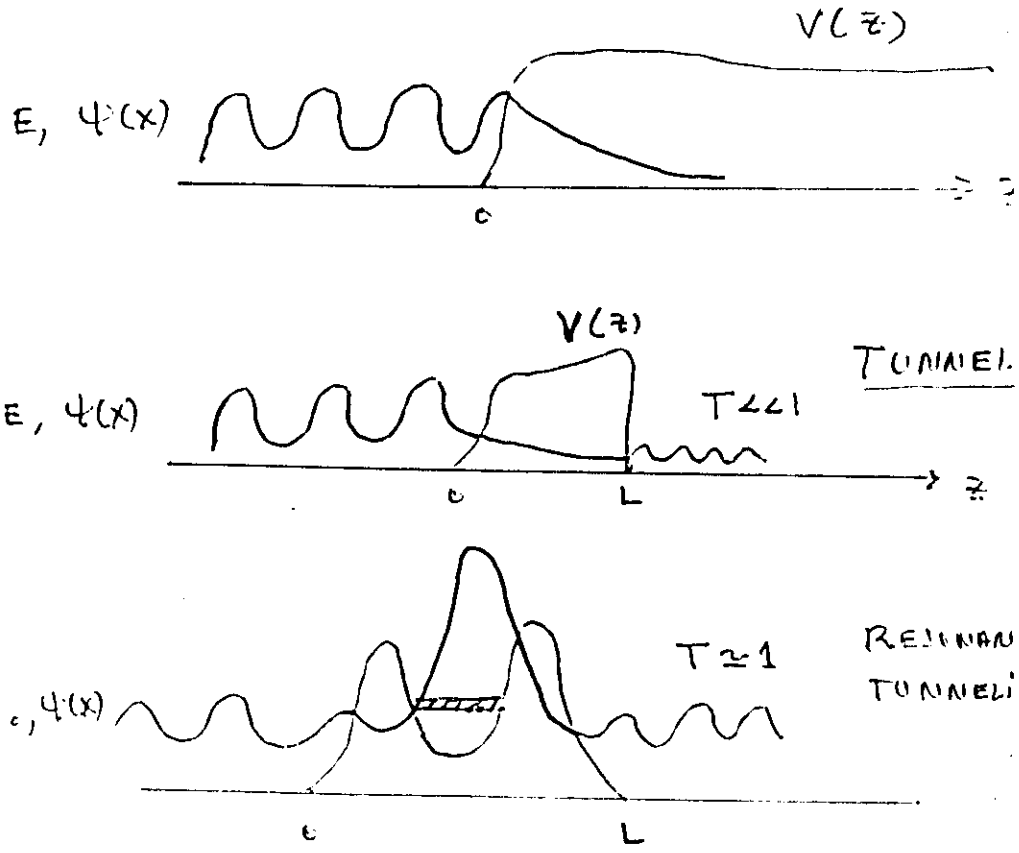
TUNNELING

OUTLINE

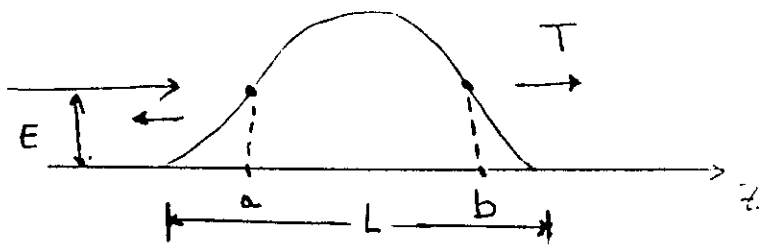
- CONCEPT OF TUNNELING
- Brief historical Sketch
- Physics of resonant tunneling Breit-wigner description of resonances. Elastic and inelastic effects. Current-voltage characteristics
- Tunneling times. The decay time. The dwell time. The Phase transmission time.

CONCEPT OF TUNNELING

- Natural consequence of Q.M.
- Wave-like properties of Matter
- $\psi(x) \neq 0$ in classically forbidden region



WKB Approximation



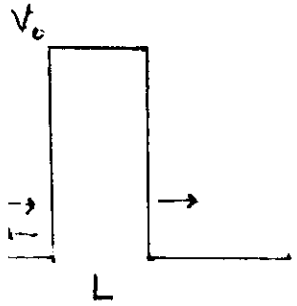
$$T \sim \exp\left[-2\int_a^b K(z)\,dz\right]$$

$$K(z) = \sqrt{\frac{2m}{\hbar^2}\left[V(z)-E\right]} \quad ; \quad \boxed{L \gg \lambda}$$

validity

$$\lambda = \frac{\lambda}{p}$$

Example:



$$T^{WKB} \sim A \exp\left\{-\frac{2}{\hbar}\sqrt{2m(V_0-E)}\,L\right\}$$

$$\frac{1}{\hbar}\sqrt{2mE}$$

$$T^{EXACT} = \frac{1}{\left[1+\frac{1}{4}\left(\frac{q}{k}-\frac{k}{q}\right)^2 \sinh^2 qL\right]}$$

$$\frac{1}{\hbar}\sqrt{2m(V_0-E)} \qquad \boxed{\frac{1}{\hbar}\sqrt{2m(V_0-E)}\,L \gg 1} \; ; \; T^{EXACT} = T^{WKB}$$

Brief Historical Sketch

Following Max Born's interpretation of ψ (1925–1927)

1928 consideration of tunneling in 3 different phenomena

- Natural radioactive decay of α-particles in certain heavy nuclei

  G. Gamow, Z. Phys. 51, 204 (1928)

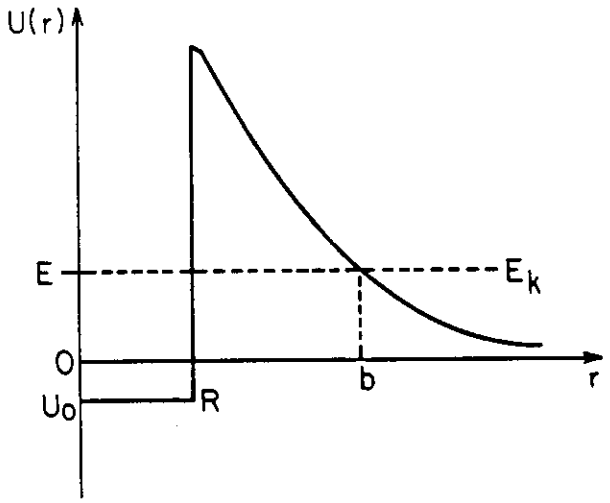
- Ionization of atomic hydrogen in a strong electric field

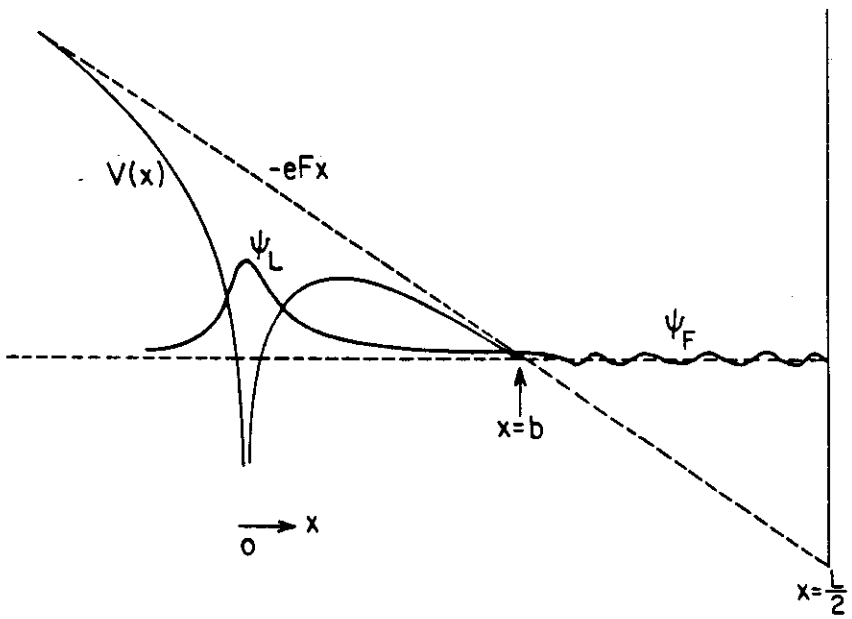
  J.R. Oppenheimer, Phys. Rev. 31, 66 (1928)

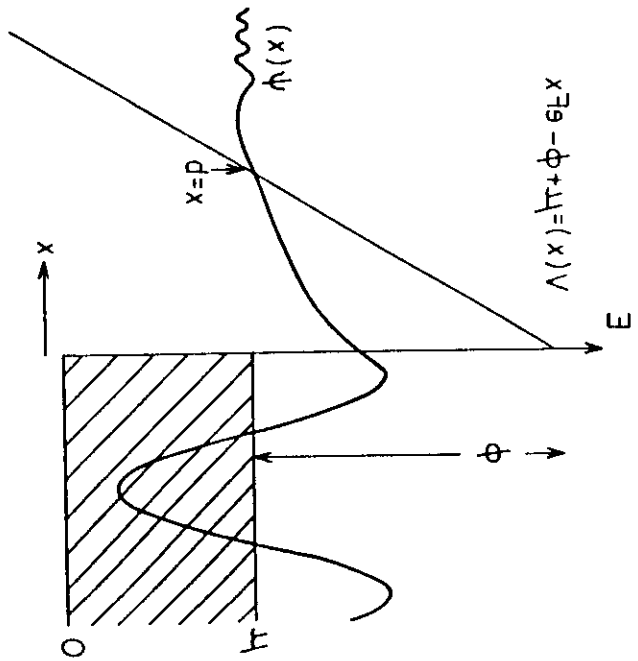
- Field emission of electrons from metal

  R.H. Fowler & L. Nordheim

  Proc. Phys. Soc. (London) A119, 173 (1928)


U(r)
E
E_k
0
U_0
R
b
r


V(x)
-eFx
ψ_L
ψ_F
x=b
0
x
$x=\frac{L}{2}$



Tunneling in Solids

a) Interband tunneling in one and the same semiconductor i.e. tunnel diode.

b) tunneling in structures involving a combination of different materials i.e. Metal – Insulator – metal (M-I-M)

Tunnel diode (Esaki, 1958)

Technological improvements:

- Grown of high quality single crystals of Ge and Si.
- Construction of p-n junction (Alloy junction method)

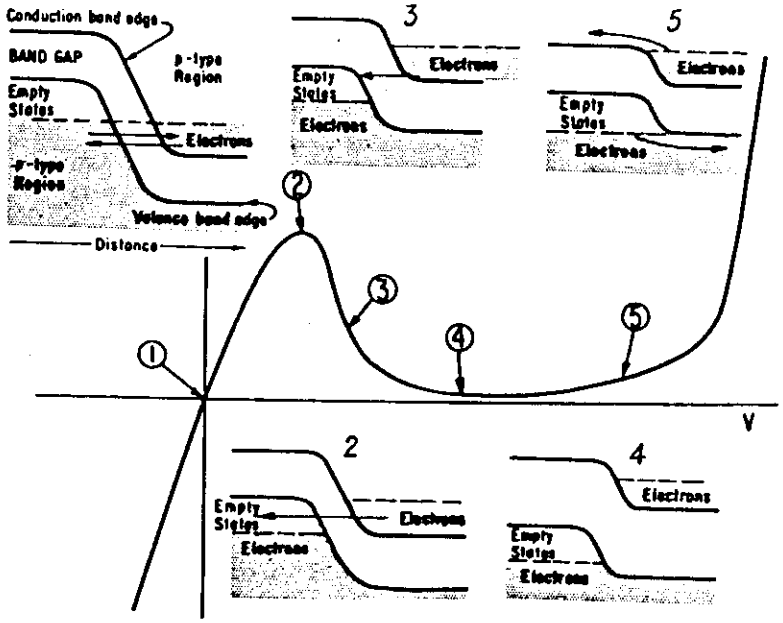
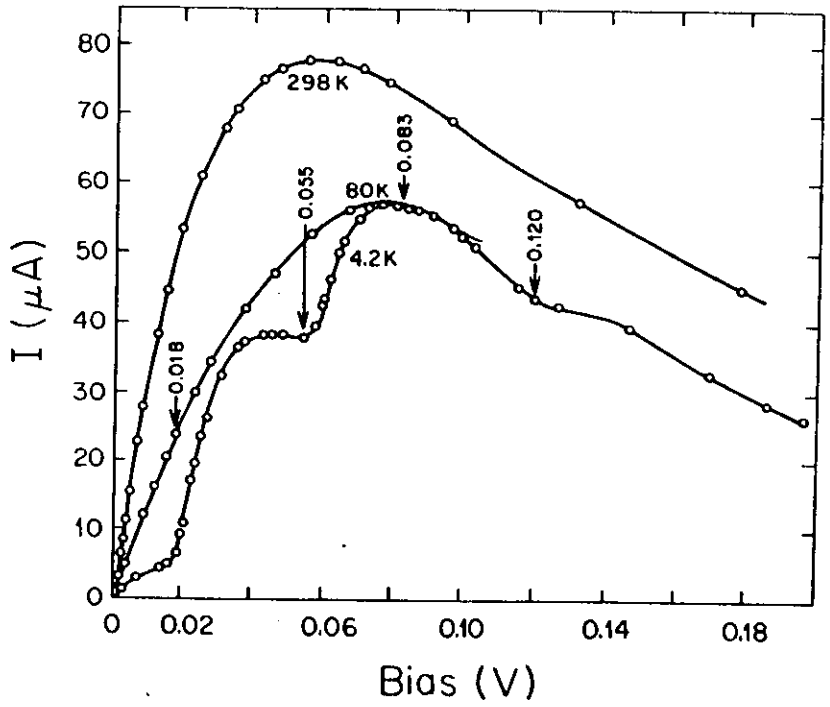


Fig. 11. Schematic illustration of current–voltage characteristic in the tunnel diode.



(1960) 1961)

FIG. 15. (a) Schematic illustration of a planar metal-insulator-metal tunnel junction. In an actual junction, the insulator thickness is about 20–30 A, whereas the metal electrodes are usually films that are thousands of angstroms thick. (b) The potential energy versus distance in the junction shown in Fig. 15a when the applied bias, V, is zero. (c) The potential energy versus distance in the junction shown in Fig. 15a when the applied bias is V.

Both Esaki and Giaever shared with Josephson the 1973 Nobel Prize in Physics.

Important aspects

- construction of reproducible solid-state structures
- Importance of I–V characteristics to learn about the electronic properties of the solid-state structure
- relevance for both science and technology of man-made solid state structures.

1969

— C.B. Duke, "Tunneling in Solids"
Academic Press, 1969

— E. Burstein & S. Lundqvist,
"Tunneling Phenomena in Solids"
Plenum Press, 1969

1984

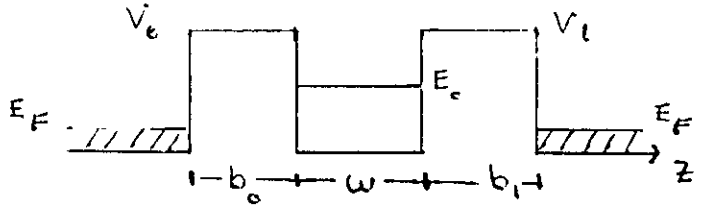
— E.L. WOLF, "Principles of Electron
Tunneling Spectroscopy"
Oxford University Press, 1985

Inventions based on tunneling
1986 Nobel Prize in Physics:
- Electron Microscope; Ruska
- Scanning tunneling Microscope; Binnig and Rohrer

Resonant Structures

1970 – 1974; Esaki, Tsu, Chang

Finite number of alternating layers of $Ga_{1-x}Al_xAs$ and GaAs giving origin to a one-dimensional potential profile.



Possibility of controlling
heights: V_0, V_1
barrier widths: b_0, b_1
well width: w
Number of barriers and wells.

Model: Tsu & Esaki, Appl. Phys. Lett. 22, 562 (1973)

- Effective mass approximation
- Due to one dimensional potential profile, Schrödinger equation is separated in 2 components, parallel and perpendicular to the interface

$$\psi = \psi_z \psi_{\parallel}$$

$$E = E_z + \frac{\hbar^2 k_{\parallel}^2}{2m^*}$$

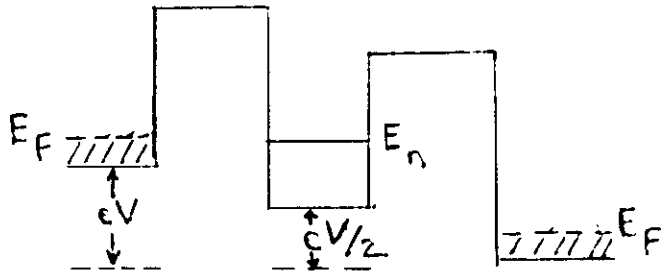
- Total energy is and momentum parallel to the interface are conserved
- Process is coherent i.e. $\lambda_B > L$ $\lambda_B = \frac{h}{p}$ de Broglie wavelength, L, system length

Tunneling Current

Connection with experiment:

Applied voltage

- Field is uniformly distributed



Current: $I = I_{LR} - I_{RL}$

$$I_{LR} = \frac{e}{4\pi^2\hbar} \int dE_z\, d^2k_{\parallel}\, f(E, k_{\parallel}) \left[1 - f(E+eV, k_{\parallel})\right] T(E_z)$$

$$I_{RL} = \frac{e}{4\pi^2\hbar} \int dE_z\, d^2k_{\parallel}\, f(E+eV, k_{\parallel}) \left[1 - f(E, k_{\parallel})\right] T(E_z)$$

$$I = \frac{e}{4\pi^3\hbar} \int dE_z\, d^2k_\parallel \left[f(E, k_\parallel) - f(E+eV, k_\parallel) \right] T(E_z)$$

$$I = \frac{e\, m^* k_B \theta}{2\pi^2 \hbar^3} \int dE_z\, T(E_z)\, \ln \left\{ \frac{1 + \exp\left[(E_F - E_z)/k_B\theta\right]}{1 + \exp\left[(E_F - E_z - eV)/k_B\theta\right]} \right\}$$

θ, Temperature; k_B, Boltzmann constant.

Low T :

$$I = \frac{e m^*}{2\pi^2 \hbar^3} \left[V \int_0^{E_F - eV} dE_z\, T(E_z) + \int_{E_F - eV}^{E_F} (E_F - E_z)\, T(E_z)\, dE_z \right] ; \quad eV \leq E_F$$

$$I = \frac{e m^*}{2\pi^2 \hbar^3} \int_0^{E_F} dE_z\, (E_F - E_z)\, T(E_z) \quad ; \quad eV > E_F$$

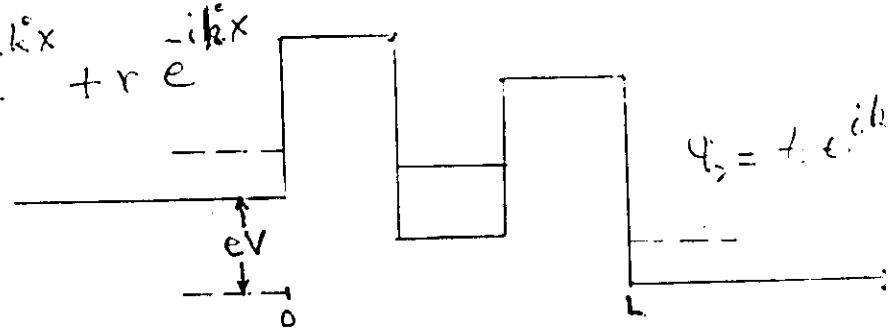
In order to obtain $T(E_z)$

1-D Schrödinger eq.

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + V(z) - E \right] \psi_E(z) = 0$$

$V(z)$ potential profile

$$\psi_L = e^{ikx} + r\, e^{-ikx}$$



$$\psi_R = t\, e^{ikx}$$

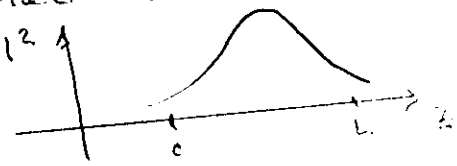
Transfer Matrix : matching of ψ_z at each bar (i.e. interface)

$$\begin{pmatrix} t \\ 0 \end{pmatrix} = M \begin{pmatrix} 1 \\ r \end{pmatrix}$$

$$M = M_1 \cdots M_n \quad ; \quad M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

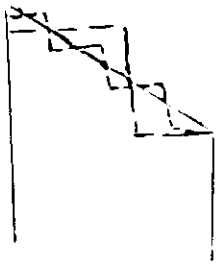
$$r = -\frac{M_{21}}{M_{22}} \qquad t = \frac{t}{M_{22}}$$

- Notice knowledge of t_i and r_i implies knowledge of the coefficients of ψ in the different potential regions. Hence $\psi_E(x)$ along the structure may be also obtained by this technique.



- Transfer matrix method can be generalized to profiles of arbitrary shape.

Example:



T.M. - Esaki, P.R.L. 23, 562 (1973)

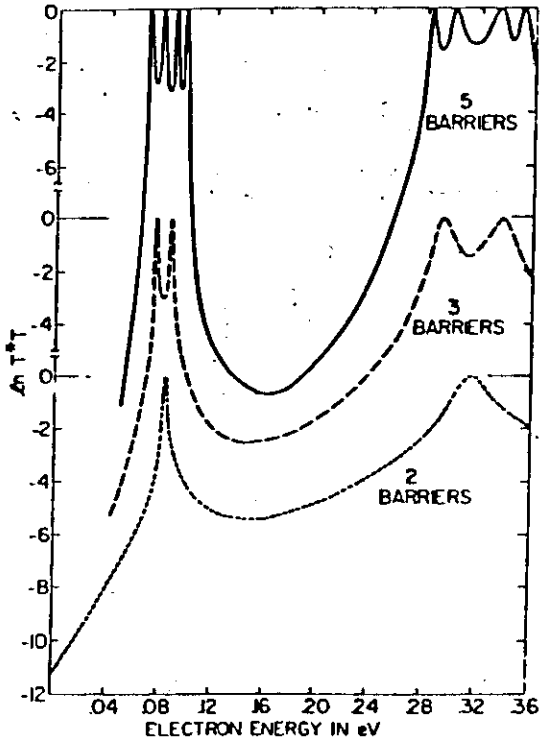


FIG. 2. Natural log of the transmission coefficient vs the electron energy in eV for the cases of a double-, triple-, and a quintuple-barrier. The barrier and well widths are 20 and 50 Å, respectively. The barrier height is 0.5 eV.

Tsu & Esaki, A.P.L. 22, 562 (1973)

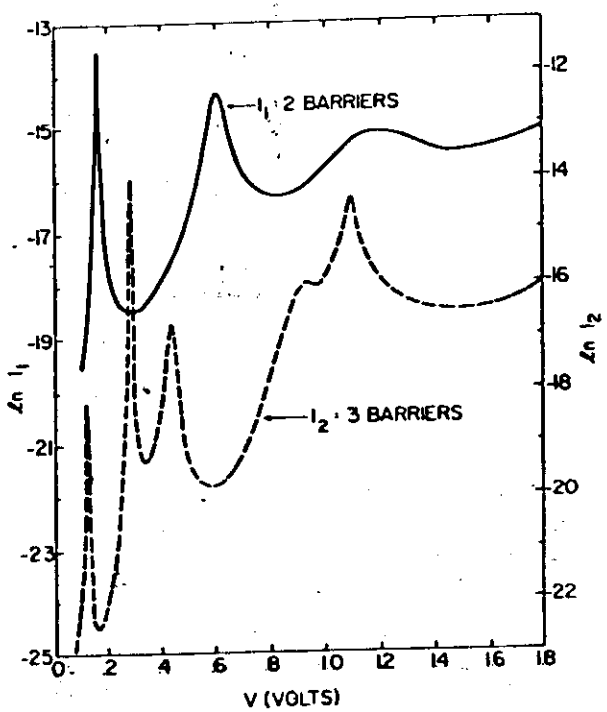


FIG. 3. Natural log of the current density $[J(em^*/2\pi^2\hbar^2)^{-1}(1.6\times10^{-12})^2]$ vs the applied voltage V. I_1 and I_2 refer to the cases of a double- and triple-barrier, respectively.

Experiment Chang, Esaki, Tsu
Appl. Phys. Lett. 24, 593 (19

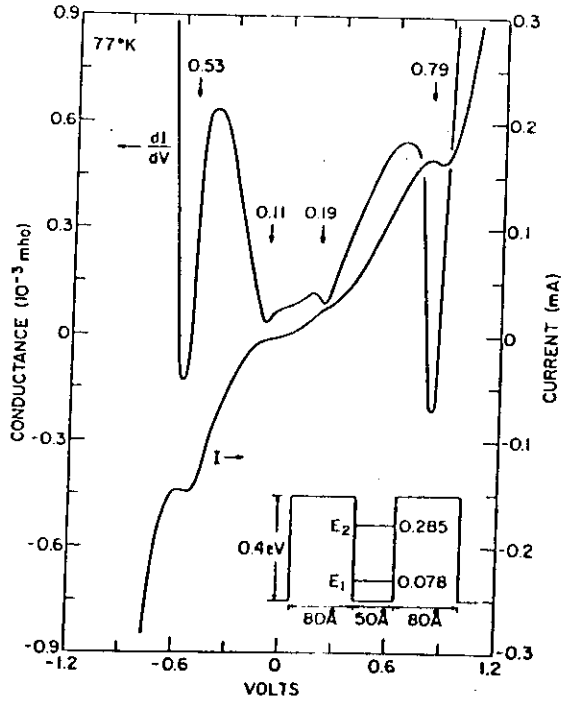


FIG. 1. Current and conductance characteristics of a double-barrier structure of GaAs between two $Ga_{0.3}Al_{0.7}As$, as shown in the energy diagram. Both the thicknesses and the calculated quasistationary states of the structure are indicated in the diagram. Arrows in the curves indicate the observed voltages of singularities corresponding to these resonant states.

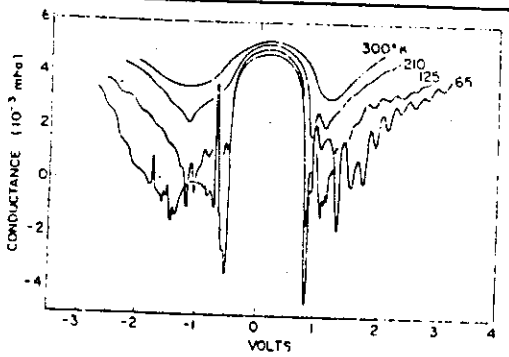


FIG. 2. Differential conductance versus applied voltage in a superlattice at four specified temperatures.

fine structure. The oscillatory behavior is observable at 210°K and becomes increasingly pronounced at lower temperatures. On the other hand, both the conductance near zero bias and a threshold voltage where the conductance begins to drop sharply are relatively insensitive to the temperature variation. Instabilities sometimes exist in the negative-conductance range which give rise to spurious conductance curves. The asymmetric characteristic with respect to polarity, as seen in Fig. 2, is fairly common in many specimens, and is likely due to an asymmetry in the potential profile, although its origin is not clear at this moment. In measuring over 20 specimens, the general features of the conductance, however, are quite reproducible: The on-

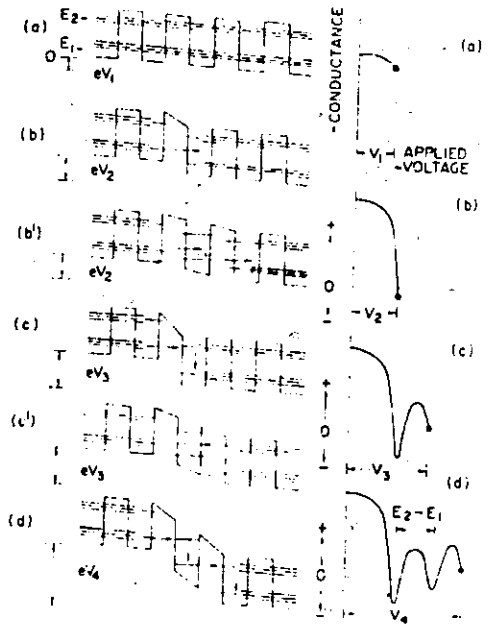
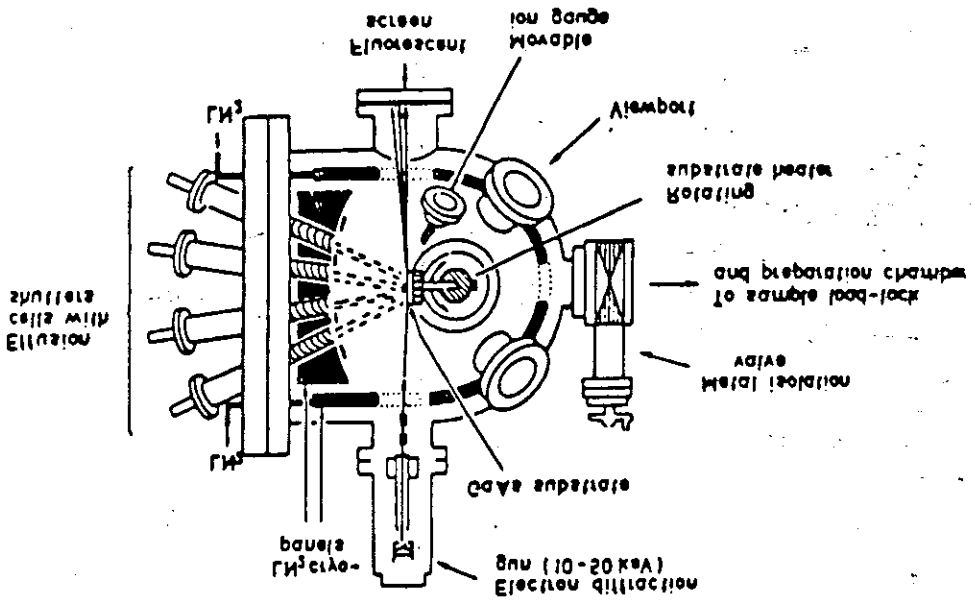


FIG. 3. Schematic energy diagrams (left-hand side) and corresponding conductances (right-hand side): (a) band conduction; (b) and (b') spontaneous generation of a domain; (c), (c'), and (d) development of domain expansion.

the total voltage will be applied across it. This will leave intact the band conduction in the rest of the superlattice region. It is also



PHYSICS OF REDUCED DIMENSIONALITY
QUANTUM WELLS
SUPERLATTICES

DEVICE PHYSICS

HETERO-INTERFACE PHYSICS

[ENGINEERED STRUCTURES]

DEVICES:
MODFET
MQW LASERS
APD . RST
Hetero-Bipolars

MATERIAL SCIENCE:
MBE
MOCVD
....

[COMPOUND SEMICONDUCTORS]

Sollner et al. Appl. Phys. Lett. 43, 588 (1983)

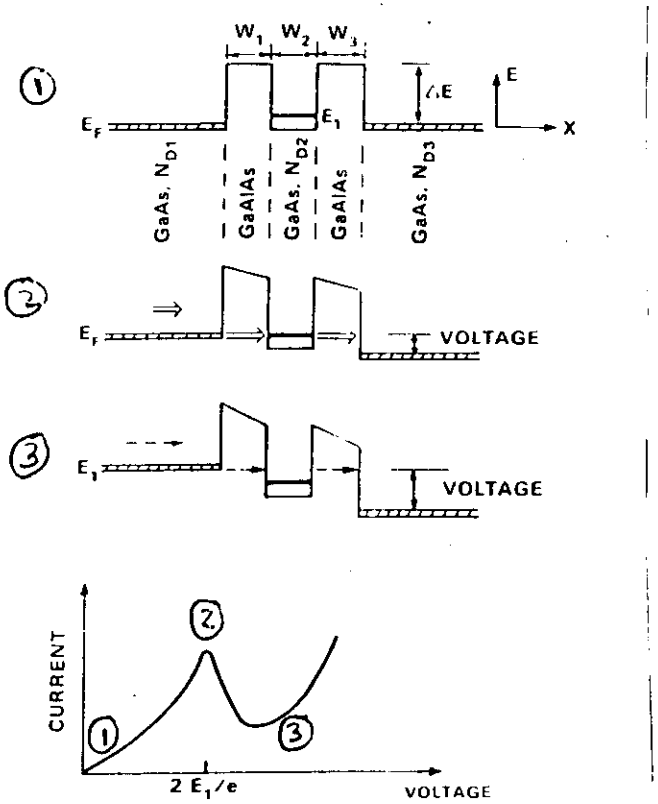


FIG. 1. Electron energy as a function of position in the quantum well structure. The parameters are $N_{D1} = N_{D3} = 10^{18}$ cm^{-3}, $N_{D2} = 10^{17}$ cm^{-3}, and $W_1 = W_2 = W_3 = 50$ Å. The doping level in the well center is an average value achieved by placing a layer of 10^{18} cm^{-3} material in the central 10% of the well. The energy level E_1 occurs above the bottom of the bulk conduction band because of confinement in the x direction. From the aluminum concentration ($x \simeq 25\%$–30%) we estimate $\Delta E = 0.23$ eV.

Sollner et al. Appl. Phys. Lett. 43, 588 (1983)

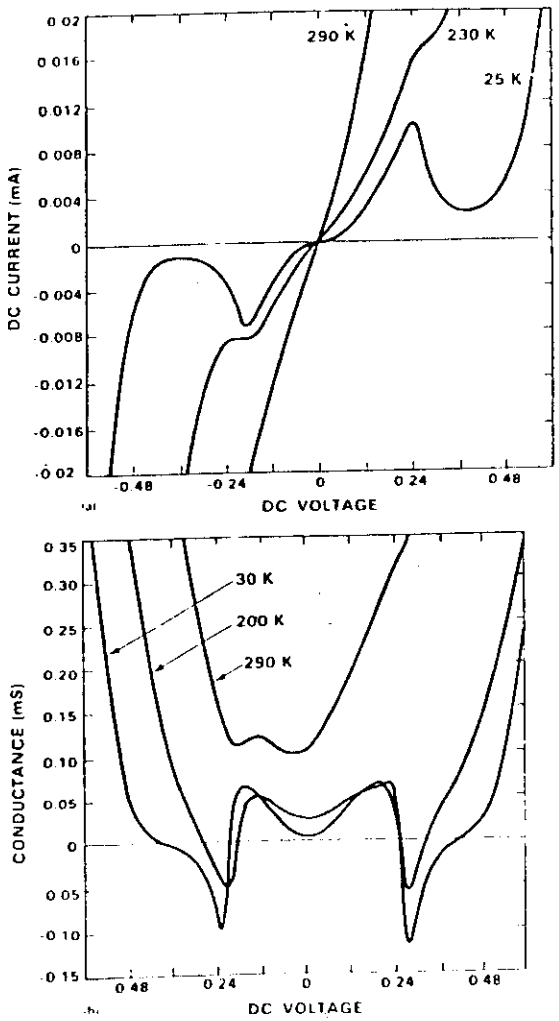


FIG. 2. (a) Current-voltage and (b) conductance [dI/dV]-voltage curves at three temperatures. Notice that resonant tunneling features can be seen even at room temperature.

Goodnick et al. J. Appl. Phys. 66, 278 (1989)

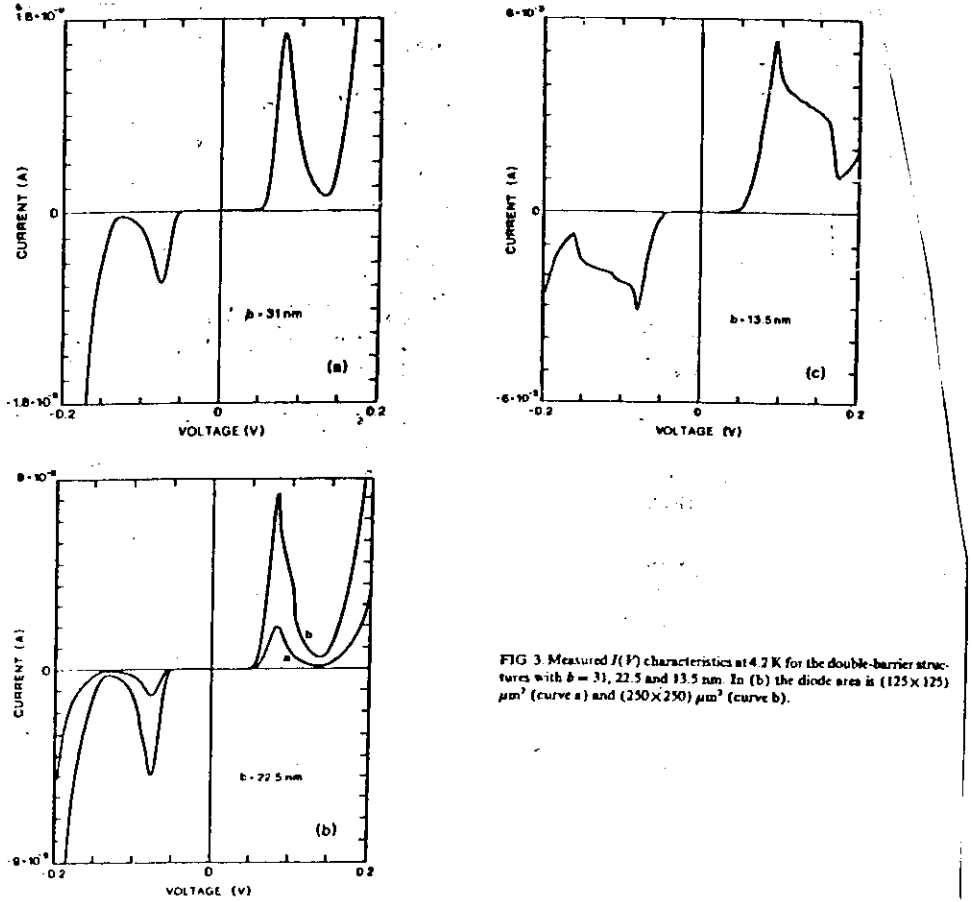
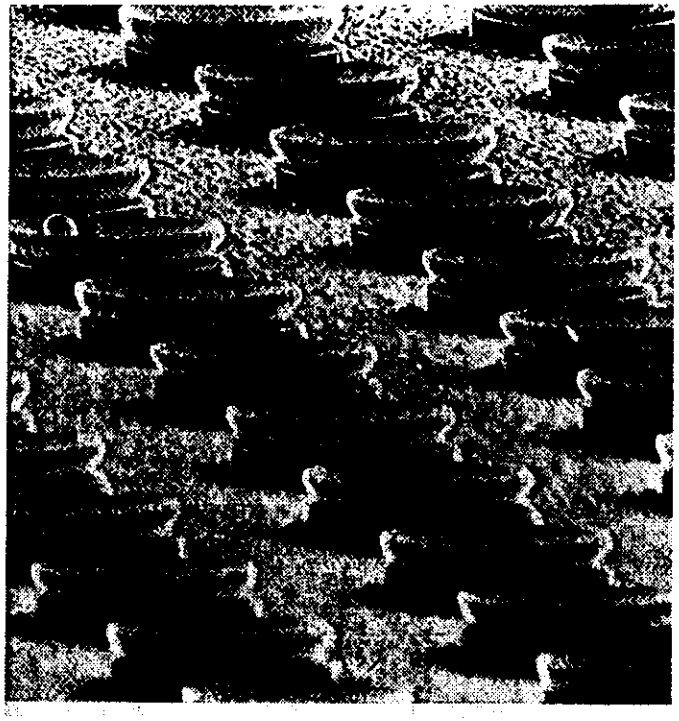
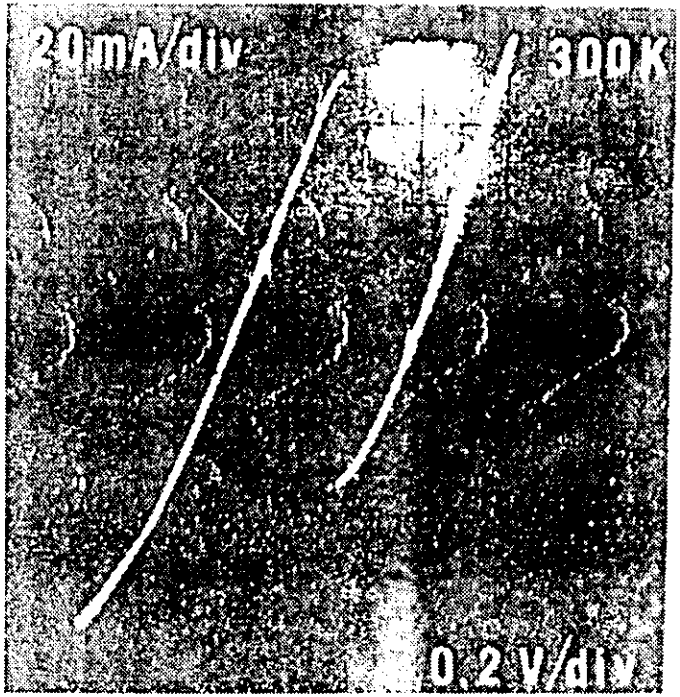


FIG. 3. Measured $I(V)$ characteristics at 4.2 K for the double-barrier structures with $b = 31$, 22.5 and 13.5 nm. In (b) the diode area is (125×125) μm^2 (curve a) and (250×250) μm^2 (curve b).



Electron micrograph of an array of resonant tunneling diodes.

(G. Sollner and coworkers at MIT Lincoln Labs).



Current voltage characteristics of diode

at room temperature

1973 – 1983

Improvement in the quality of experimental results. (Better materials, etc.

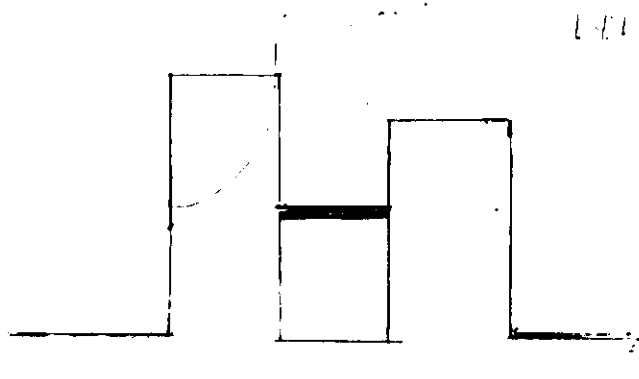
confrontation of TSU – Esaki Theoretical model with experiment.

Physics of Resonant tunneling

Ricco & Azbel, Phys. Rev. B 29, 1970 (1984)

emphasize:

- Effect of applied voltage on resonances
- Time aspects of resonances (width)
- Effects of space charge in modifying potential profile
- Temperature effects.



$$T = \frac{C_i}{C_1 T_l T_r + C_2 \frac{T_l}{T_r} + C_3 \frac{T_r}{T_l} + C_4 \frac{1}{T_l T_r}}$$

T_l, left barrier

T_r, right barrier

C_i, phase functions, ~ constant to 1st order ~ same magnitude.

- Sharp resonance requires: $T_l, T_r \ll 1$
- dominant terms $C_4 \frac{1}{T_l T_r}$;

$$T \sim \frac{C_i}{C_4} T_l T_r \ll 1$$

However, at certain energies: $C_4 = 0$

(resonance energy)

$$T \approx \frac{c_0}{c_2 \frac{T_l}{T_r} + c_3 \frac{T_r}{T_l}}$$

denote T_{min}, T_{max} smaller and larger, respectively, of T_l and T_r

$$\boxed{T \simeq c \, \frac{T_{min}}{T_{max}}}$$

noticed $T_l = T_r$

$$\boxed{T = 1}$$

$$c = \frac{c_0}{c_2} \text{ or } \frac{c_0}{c_3}$$

Then

$$\begin{cases} T^{off} \sim T_{min} T_{max} \\ T^{res} \sim \dfrac{T_{min}}{T_{max}} \end{cases}$$

$$\boxed{\frac{T^{res}}{T^{off}} \sim \frac{1}{T_{max}^2}}$$

$$\boxed{\Gamma \propto T_{max}}$$

[illegible]

Γ, width

- $$I_{res} \propto \left(\frac{T_{min}}{T_{max}}\right) T_{max} \propto T_{min}$$

($\frac{T_{min}}{T_{max}}$: transmission at resonance; T_{max}: fraction of electrons involved at resonance)

- $$I_{off} \propto \left(T_{max} T_{min}\right) T_{max} \sim T_{max}^2 T_{min}$$

($T_{max} T_{min}$: transmission off resonance)

$$\boxed{\frac{I_{res}}{I_{off}} \simeq \frac{1}{T_{max}^2}}$$

may give extremely large current increase.

Example

From Tsu & Esaki, Appl. Phys. Lett. 22, 562 (1973)

numerical calculation (Fig. 3)

$$\frac{J_{res}}{J_{off}} \simeq 1.6 \times 10^4$$

$V_0 = .5$ eV

$E_r \simeq .06$ eV

d (barrier) $= 20$ Å

assuming $m^* = .1\, m_e$

$$\frac{J_{res}}{J_{off}} \simeq \frac{1}{T_{max}} = \left[\frac{V_1^2}{4(V_1 - E)E}\right]^2 \exp\left[4\sqrt{\frac{2m^*}{\hbar^2}(V_1 - E)}\, d\right]$$

$$\frac{J_{res}}{J_{off}} \simeq 10^3$$

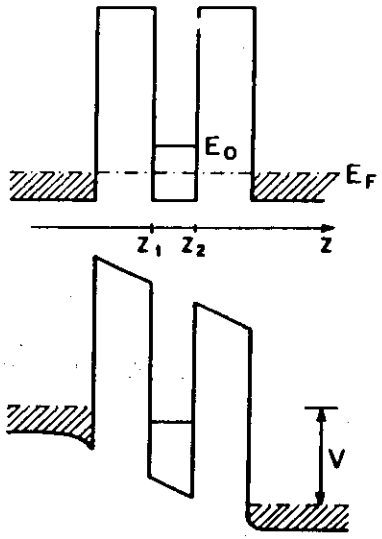
In any case large compared with experimental results.

S. Luryi, Appl. Phys. Lett. 47, 490 (1985)

- Non-linear behaviour of I vs V i.e. existence of negative differential resistance does not require coherence of the electron wave function.
- Coherent tunneling is sufficient but not necessary to achieve NDR.
- NDR arises simply from energy and momentum ($k_{\parallel}$) conservation considerations.
- NDR follows from reduction in the dimensionality of the electron states.

3D (emitter) → 2D (well)

S. Luryi, Appl. Phys. Lett. 47, 490 (1985)



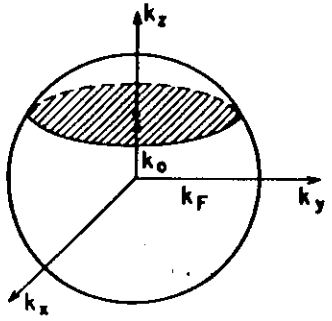
Emitter

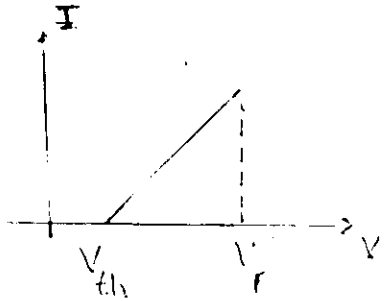
$$E_{3D} = E_z + \frac{\hbar^2 k_{\parallel}^2}{2m^*}$$

$$k_{\parallel}^2 = k_x^2 + k_y^2$$

well

$$E_{2D} = E_0 + \frac{\hbar^2 k_{\parallel}^2}{2m^*}$$

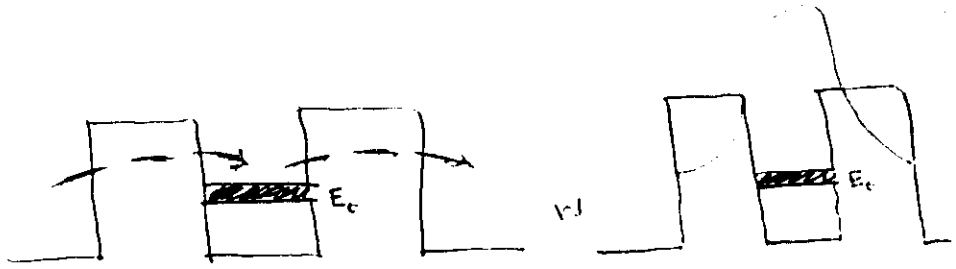




conservation of E and $k_{\parallel}$

$\Rightarrow$ $E_z = E_0$ i.e. $\boxed{k_0 = k_z}$

- Luryi also suggested other mechanisms for tunneling, i.e., sequential tunneling.



Sequential

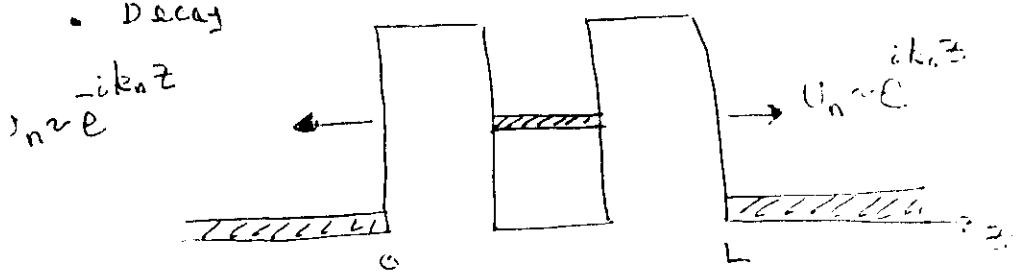
coherent

implies according to Luryi

- Smaller peak to valley ratio than for fully coherent tunneling
- Peak current less sensitive to the asymmetry of structure.

Resonance formalism

- Definition of resonant or quasi-bound state. coherent (elastic).
- arbitrary potential profile
- Decay



(power outgoing waves through both channels)

Solutions of Schrödinger eq.

$$U_n''(z) + \left[k_n^2 - V(z)\right] U_n(z) = 0$$

boundary conditions

$$\begin{cases} \dfrac{U_n'(0_+)}{U_n(0_+)} = -ik_n \\ \dfrac{U_n'(L_-)}{U_n(L_-)} = ik_n \end{cases}$$

Important Physical requirement:

Equation of continuity

$$i\frac{\partial}{\partial t} U_n(z,t) = H\, U_n(z,t)$$

with $H = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z)$; $V(z)$ potential profile

$$\boxed{\frac{\partial}{\partial t}|U_n|^2 + \frac{\partial}{\partial z} J_n = 0}$$

where $J_n = \frac{\hbar}{2mi}\left[U_n^* \frac{\partial}{\partial z} U_n - U_n \frac{\partial}{\partial z} U_n^*\right]$

one may write, integrating:

$$\boxed{\frac{\partial}{\partial t}\int_0^L |U_n(z,t)|^2 dz = J_n(0,t) - J_n(L,t)}$$

notice: $J_n = \frac{\hbar}{2mi}|U_n|^2\left[\frac{U_n'}{U_n} - \frac{U_n'^*}{U_n^*}\right]$

$$J_n(z,t) = \frac{\hbar}{m}|U_n(z,t)|^2\, \mathrm{Im}\left(\frac{U_n'}{U_n}\right)$$

$$\frac{\partial}{\partial t}\int_0^L |U_n(z,t)|^2 dz = \frac{\hbar}{m}|U_n(0,t)|^2 \operatorname{Im}\left(\frac{U_n'(0)}{U_n(0)}\right) - \frac{\hbar}{m}|U_n(L,t)|^2 \operatorname{Im}\left(\frac{U_n'(L)}{U_n(L)}\right)$$

- Can k_n be real? let $k_n = b_n$, b_n real $\neq 0$

In that case $\begin{cases} \dfrac{U_n'(0)}{U_n(0)} = -ib_n \\ \dfrac{U_n'(L)}{U_n(L)} = ib_n \end{cases}$

$$|U_n(z,t)|^2 = |U_n(z)|^2$$

$$0 = -\frac{\hbar}{m}\left[|U_n(0)|^2 + |U_n(L)|^2\right] b_n$$

$\Rightarrow$ $b_n = 0$ or $|U_n(0)|^2 = |U_n(L)|^2 = 0$

hence real eigenvalues do not fulfill the physical requirement of a constant probability flux $\hbar/m$ through each channel.

- let $k_n = i\gamma_n$ (purely imaginary)

$$\frac{U_n'(0)}{U_n(0)} = -ik_n = \gamma_n$$

$$\frac{U_n'(L)}{U_n(L)} = ik_n = -\gamma_n$$

: no prob. current.

- let $k_n = a_n - ib_n$ (complex)

$$\begin{cases} \operatorname{Im}\left(\dfrac{U_n'(0)}{U_n(0)}\right) = -a_n \\ \operatorname{Im}\left(\dfrac{U_n'(L)}{U_n(L)}\right) = a_n \end{cases}$$

$$|U_n(z,t)|^2 = |U_n(z)|^2 \, e^{-\Gamma_n t/\hbar}$$

$$E_n = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2}{2m}(a_n^2 - b_n^2) - i\frac{\hbar^2}{2m}2a_n b_n$$

$$E_n = \mathcal{E}_n - i\Gamma_n/2$$

$$\int_0^L |U_n(z)|^2 dz \left(-\frac{\Gamma_n}{\hbar}\right) e^{-\Gamma_n t/\hbar} = -\left(\frac{\hbar}{m}a_n\right)|U_n(0)|^2 e^{-\Gamma_n t/\hbar}$$

$$\Gamma_n = \frac{2\hbar a_n}{m}|U_n(0)|^2 e^{-\Gamma_n t}$$

$$\Gamma_n = \Gamma_n^0 + \Gamma_n^L$$

Γ_n elastic decay width

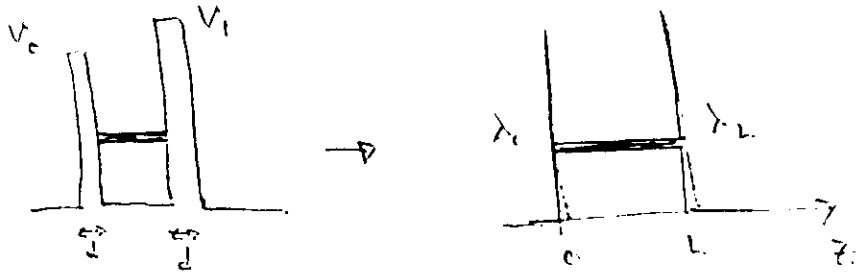
Γ_n^0, Γ_n^L partial decay widths

$$\Gamma_n^0 = \hbar\left(\frac{\hbar a_n}{m}\right)\frac{|U_n(0)|^2}{\int_0^L |U_n(z)|^2 dz}$$

$$\Gamma_n^L = \hbar\left(\frac{\hbar a_n}{m}\right)\frac{|U_n(L)|^2}{\int_0^L |U_n(z)|^2 dz}$$

Partial decay widths show explicitly a coherent nature of resonant states

Example complex eigenvalue eq.



$V_0 d \to \lambda_0$; $V_1 d \to \lambda_L$ | $\lambda_0, \lambda_L \to \infty$

$V_0 \to \infty$, $d \to 0$; $V_1 \to \infty$, $d \to 0$ | Box

$$k_n = \frac{n\pi}{L}$$

$$U_n''(z) + \left[k_n^2 - V(z)\right] U_n(z) = 0$$

$$V(z) = \lambda_0 \delta(z) + \lambda_L \delta(z-L)$$

Solutions

$$\begin{cases} U_n(z) = C_n e^{-ik_n z} & ; \ z \le 0 \\ U_n(z) = A_n e^{ik_n z} + B_n e^{-ik_n z} & ; \ 0 \le z \le L \\ U_n(z) = D_n e^{ik_n z} & ; \ z \ge L \end{cases}$$

Continuity at x = 0 and x = L

$$\text{①}\begin{cases} U_n'(0_+) - U_n'(0_-) = \lambda_0 U_n(0) \\ U_n(0_+) - U_n(0_-) = 0 \end{cases}$$

$$\text{②}\begin{cases} U_n'(L_+) - U_n'(L_-) = \lambda_L U_n(L) \\ U_n(L_+) - U_n(L_-) = 0 \end{cases}$$

$$\text{①}\begin{cases} A_n = \dfrac{\lambda_0}{2ik_n} C_n \\ B_n = \dfrac{2ik_n - \lambda_0}{2ik_n} C_n \end{cases}$$

$$U_n(x) = C_n \left[\frac{\lambda_0}{2ik_n} e^{ik_n x} + \frac{2ik_n - \lambda_0}{2ik_n} e^{-ik_n x} \right]$$

$$\text{②}\begin{cases} A_n = \dfrac{2ik_n - \lambda_L}{2ik_n} D_n \\ B_n = \dfrac{\lambda_L}{2ik_n} e^{2ik_n L} D_n \end{cases}$$

eigenvalue equation:

$$(2ik_n)^2 - 2ik_n(\lambda_0 + \lambda_L) + \lambda_0\lambda_L\left(e^{2ik_n L} - 1\right) = 0$$

$$\frac{(2ik_n)^2}{\lambda_0\lambda_L} - 2ik_n \frac{\lambda_0 + \lambda_L}{\lambda_0\lambda_L} + \left(e^{2ik_n L} - 1\right) = 0$$

$\lambda_0, \lambda_L \to \infty$ $\quad e^{2ik_n L} - 1 = 0$

$$k_n = \frac{n\pi}{L}$$

Approximate Solution:

Hence; $(\lambda_0, \lambda_L) \gg 1$ but finite.

n, small

θ_n small

$k_n = a_n - ib_n$

$a_n \simeq \frac{n\pi}{L} - \theta_n$;

$$e^{2ik_n L} - 1 \simeq 2ik_n \frac{\lambda_0 + \lambda_L}{\lambda_0\lambda_L} \quad ; \quad \gamma \equiv \frac{\lambda_0 + \lambda_L}{\lambda_0\lambda_L}$$

$$e^{2b_n L}\left[\cos 2a_n L + i \sin 2a_n L - 1\right] \simeq 2i a_n \gamma + 2 b_n \gamma$$

since; $2b_n\gamma \ll 1$

③ $\quad \cos 2a_n L \, e^{2b_n L} \simeq 1$

④ $\quad \sin 2a_n L \, e^{2b_n L} \simeq 2a_n\gamma$

④/③ : $\quad \tan 2a_n L \simeq 2a_n\gamma$; $\quad 2a_n\gamma \ll 1$

$$\theta_n \simeq \frac{1}{2L} \tan^{-1}\left(\frac{n\pi}{L}\gamma\right) \simeq \frac{n\pi}{2} \frac{\gamma}{L}$$

$k_n = a_n - i b_n$

$$a_n = \frac{n\pi}{L}\left[1 - \frac{\lambda_c + \lambda_L}{L\lambda_c\lambda_L}\right]$$

on the other hand: $(\ )^2 + (\ )^2$ yields

$$e^{4k_n L} = 1 + 4a_n^2\gamma^2$$

$$b_n = \frac{1}{4L}\ln\left[1 + \frac{4n^2\pi^2}{L^2}\gamma^2\right]$$

$$b_n \simeq \frac{1}{L}\frac{n^2\pi^2}{L^2}\left(\frac{\lambda_c + \lambda_L}{\lambda_c\lambda_L}\right)^2$$

$$\varepsilon_n = \frac{\hbar^2}{2m}(a_n^2 - b_n^2) \quad ; \quad \Gamma_n = \frac{\hbar^2}{2m}2a_n b_n$$

$$\varepsilon_n \simeq \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2\left[1 - \frac{2(\lambda_c + \lambda_L)}{L\lambda_c\lambda_L}\right]$$

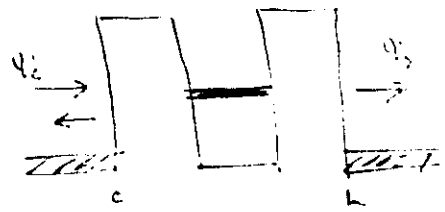
$$\Gamma_n = \frac{\hbar^2}{2m}\frac{2n^2\pi^2}{L^4}\left[\frac{1}{\lambda_c^2} + \frac{1}{\lambda_c\lambda_L}\right] + \frac{\hbar^2}{2m}\frac{2n^2\pi^2}{L^4}\left[\frac{1}{\lambda_L^2} + \frac{1}{\lambda_c\lambda_L}\right]$$

$\Gamma_n \simeq \Gamma_n' + \Gamma_n''$

connection with Scattering i.e. transmission amplitude

Green Function Calculation for bound states

$$\psi''(k,z) + [k^2 - V(z)]\psi(k,z) = 0$$



$z < 0$; $\psi_i = e^{ikz} + re^{-ikz}$

$z > L$; $\psi_t = te^{ikz}$

$$G^{+\prime\prime}(z,z';k) + [k^2 - V(z)]G^+(z,z';k) = i\hbar(\ )$$

$0 \le z' \le L$

$$\begin{cases} \left.\dfrac{\partial G^+(z,z';k)}{\partial z}\right]_{z=0_+} = -ik\,G^+(0,z';k) \\ \left.\dfrac{\partial G^+(z,z';k)}{\partial z}\right]_{z=L_-} = ik\,G^+(L,z';k) \end{cases}$$

1. $\int_0^L [\psi \times \text{eq. for } G^+ - G^+ \times \text{eq. for } \psi]\,dz$ then using the boundary conditions

2. ψ and G at $z=0$ and $z=L$

$$\psi_1^+(k,z) = 2ik\, G_1^+(0,z;k)\,; \quad 0 \le z \le L$$

$z = L$

$$t(k) = 2ik\, G_1^+(0,L;k)\, e^{-ikL}$$

$z = 0$

$$r_1(k) = 2ik\, G_1^+(0,0;k) - 1$$

condition $|t|^2 + |r|^2 = 1$

implies: **optical theorem** in 1D:

$$|G_1^+(0,L;k)|^2 + |G_1^+(0,0;k)|^2 = \frac{1}{k}\,\mathrm{Im}\, G_1^+(0,0;k)$$

Notice approaching the system from $x > L$:

$$\psi_r(k,z) = 2ik\, G_1^+(L,z;k)\, e^{-ikL}\,; \quad 0 \le z \le L$$

$$r_r(k) = \left[2ik\, G_1^+(L,L;k) - 1\right] e^{2ikL}$$

García-Calderón & Peierls

2. Nucl. Phys. B263, 443 (1976)

In one dimension:

$$G^+(z,z';k) = \frac{\psi_n(z_<)\,\psi_n(z_>)}{k^2 - k_n^2} + B(z,z';k)$$

B, background contribution, usually negligible

- residue at the complex pole provides the normalization condition for $\psi_n(z)$,

$$\int_0^L \psi_n^2(z)\,dz + \frac{i}{2k_n}\,\psi_n^2(0) + \frac{i}{2k_n}\,\psi_n^2(L) = 1$$

since

$$t = 2ik\, G_1^+(0,L;k)\, e^{-ikL}$$

$$T = |t|^2 = \frac{\Gamma_n^0\,\Gamma_n^L}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}$$

applied voltage introduces a factor $\left(\frac{k}{k_0}\right)$, but this is cancelled by similar factor in the Poisson equation [illegible] $(1/k_0)^2$

Transmission coefficient near resonance energy,

$$T(E) = \frac{\Gamma_n^0 \Gamma_n^1}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}$$

two elastic channels

$$\Gamma_n = \Gamma_n^0 + \Gamma_n^1$$

Partial decay widths control peak value.

$$T(\varepsilon_n) = \frac{4\Gamma_n^0 \Gamma_n^1}{(\Gamma_n^0 + \Gamma_n^1)^2} \quad \text{(at resonance)}$$

$\Gamma_n^0 = \Gamma_n^1$; $T(\varepsilon_n) = 1$ Full Transmission

asymmetry:

$\Gamma_n^0 << \Gamma_n^1$; $T(\varepsilon_n) \simeq \frac{4\Gamma_n^0}{\Gamma_n^1} << 1$

$\Gamma_n^0 >> \Gamma_n^1$; $T(\varepsilon_n) \simeq \frac{4\Gamma_n^1}{\Gamma_n^0} << 1$

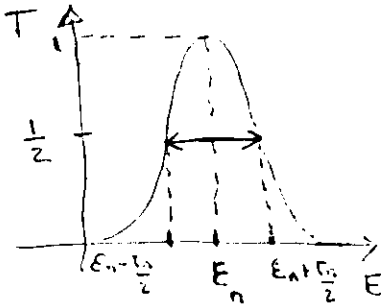
$$T(E) = \frac{\Gamma_n^0 \Gamma_n^1}{(E-\varepsilon_n)^2 + \Gamma_n^2/4} \quad ; \quad \Gamma_n = \Gamma_n^0 + \Gamma_n^1$$

For the symmetric case:

$$\Gamma_n^0 = \Gamma_n^1 = \Gamma_n/2$$

then,

$$T(E) = \frac{\Gamma_n^2/4}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}$$



Isolated sharp resonance

let $E = \varepsilon_n + \Gamma_n/2$; $T(\varepsilon_n + \Gamma_n/2) = \frac{1}{2}$

$E = \varepsilon_n - \Gamma_n/2$; $T(\varepsilon_n - \Gamma_n/2) = 1/2$

Full width at Half Maximum rule. calculation of the width (FWHM)

comment in literature one finds:

$$T(E) = \frac{\Gamma_n^2}{(E-\varepsilon_n)^2 + \Gamma_n^2}$$

$T(E_n + \Gamma_n/2) = \frac{1}{5}$

misleading if one looks for

$T(E_n - \Gamma_n/2) = 4/5$

General case

$$T(E) = \frac{\Gamma_n^0 \Gamma_n^L}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}$$

$E = \varepsilon_n + \Gamma_n/2$; $T(\varepsilon_n + \Gamma_n/2) = \frac{2\Gamma_n^0\Gamma_n^L}{\Gamma_n^2} = \frac{1}{2} T(\varepsilon_n)$

$E = \varepsilon_n - \Gamma_n/2$; $T(\varepsilon_n - \Gamma_n/2) = \frac{2\Gamma_n^0\Gamma_n^L}{\Gamma_n^2} = \frac{1}{2} T(\varepsilon_n)$

Since $T(\varepsilon_n) = \frac{4\Gamma_n^0\Gamma_n^L}{\Gamma_n^2}$ $\Rightarrow$ FWHM yields width Γ_n.

Using $\Gamma_n = \Gamma_n^0 + \Gamma_n^L$

$$\Gamma_n^0 = \frac{\Gamma_n}{2}\left[1 \mp \sqrt{R(\varepsilon_n)}\right]$$

$$\Gamma_n^L = \frac{\Gamma_n}{2}\left[1 \pm \sqrt{R(\varepsilon_n)}\right]$$

one needs to figure out the right sign!

$R(\varepsilon_n) = 1 - T(\varepsilon_n)$.

- Above procedure allows to extract resonance parameters from transmission peak, provided this is sharp and isolated and it is not very small!
- Resonance parameters may also be obtained from the complex poles of $t(E)$.

Since $t = \frac{1}{M_{2,2}}$ (transfer matrix)

complex zeros: $M_{2,2} = 0 \rightarrow \{\varepsilon_n - i\Gamma_n/2\}$

- resonant states are easily obtained by adapting transfer matrix codes to poorly outgoing waves for $z < 0$ and $z > L$.

wave functions $0 \le z \le L$

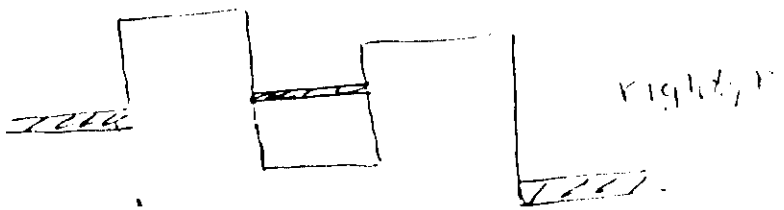
- Build up along internal region is also controlled by Γ_n^L and Γ_n^R. In fact it depends on Γ_n^L / Γ_n^R.

- For a given potential profile, in general the build up of probability density will depend on the incident direction.

$$|\psi_L(E,z)|^2 \propto \frac{\Gamma_n^L}{(E-\varepsilon_n)^2 + \Gamma_n^2/4} |\psi_n(z)|^2$$

$$|\psi_R(E,z)|^2 \propto \frac{\Gamma_n^R}{(E-\varepsilon_n)^2 + \Gamma_n^2/4} |\psi_n(z)|^2$$

left, L

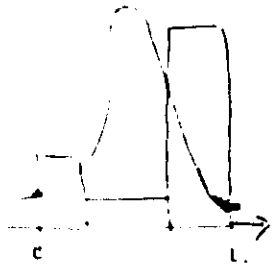


right, R

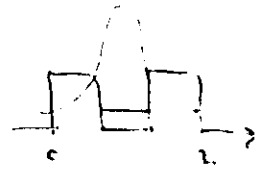
For example, approaching Resonance $z < 0$ (left), at resonance energy: $E = \varepsilon_n$

$$|\psi_L(E_n, z)|^2 \propto \frac{4\Gamma_n^L}{(\Gamma_n^L + \Gamma_n^R)^2} |\psi_n(z)|^2$$

$\Gamma_n^L \gg \Gamma_n^R$: $|\psi_L|^2 \approx \frac{|\psi_n(z)|^2}{\Gamma_n^L}$



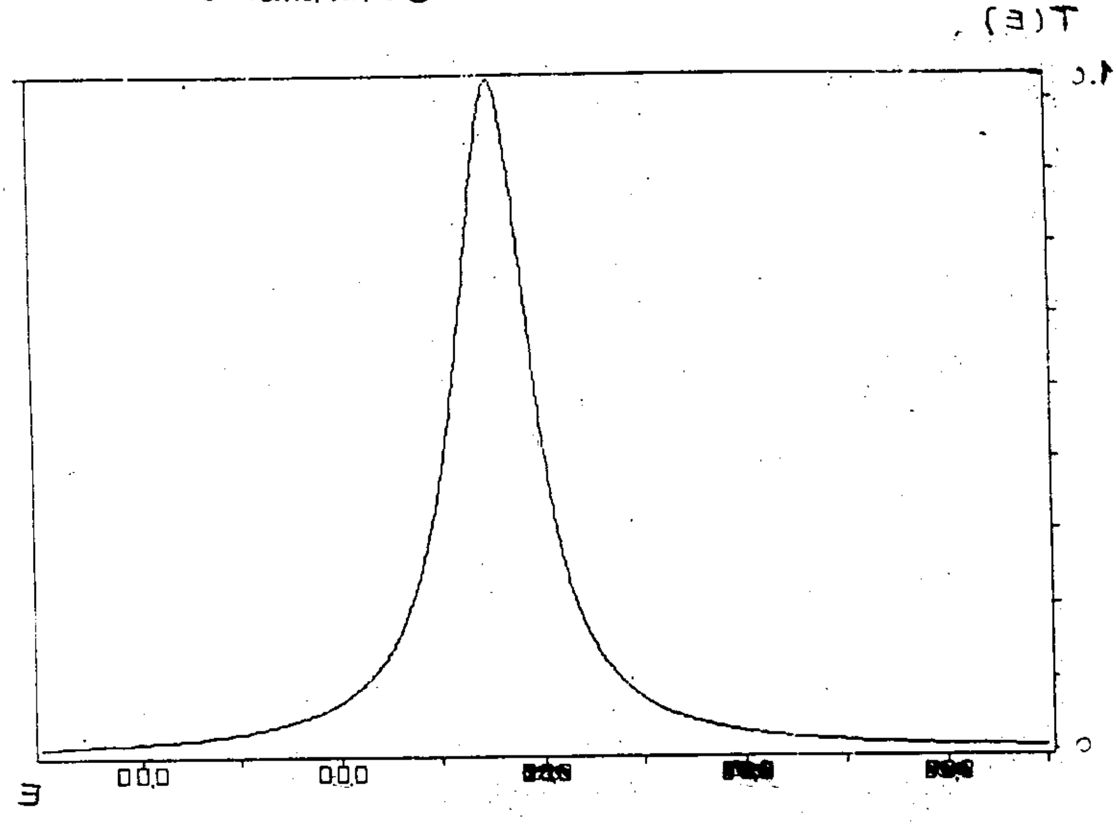
$\Gamma_n^L = \Gamma_n^R$: $|\psi_L|^2 \approx \frac{|\psi_n(z)|^2}{\Gamma_n}$



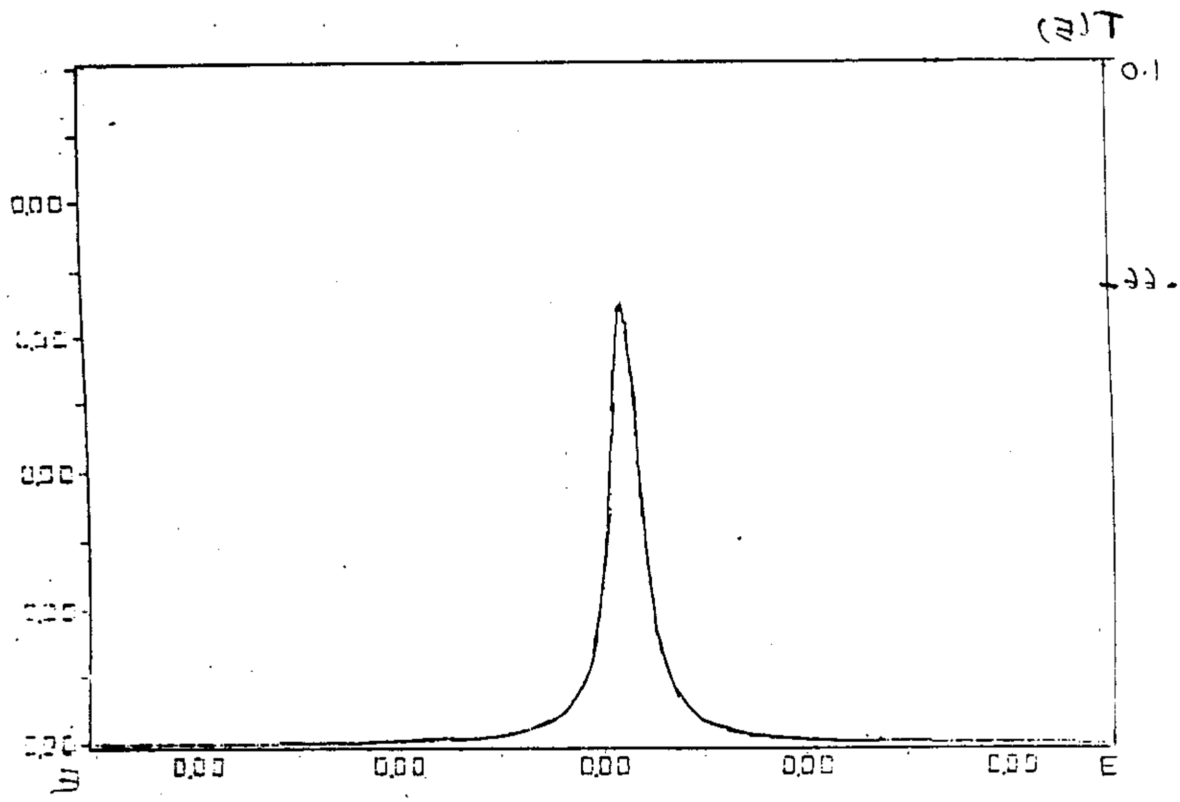
$\Gamma_n^L \ll \Gamma_n^R$: $|\psi_L|^2 \approx \left(\frac{\Gamma_n^L}{\Gamma_n^R}\right) |\psi_n(z)|^2$

- Similarly for $T(E)$.
- important for potential profile design.

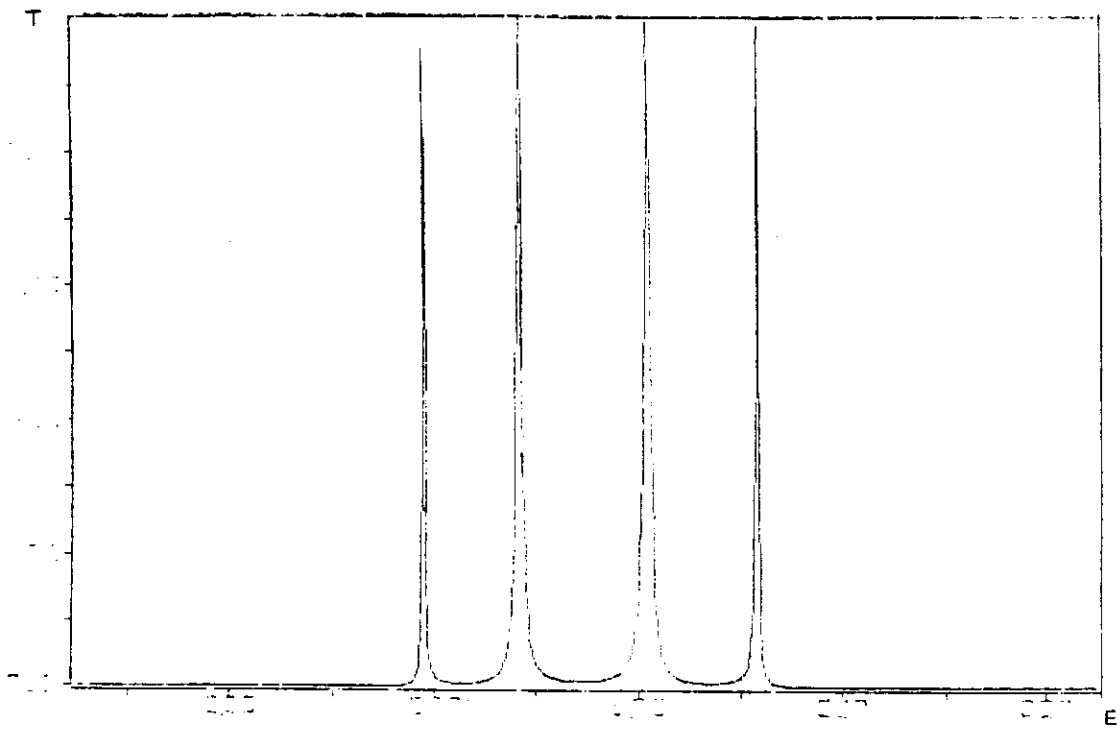
Symmetric Double barrier



Asymmetric double barrier



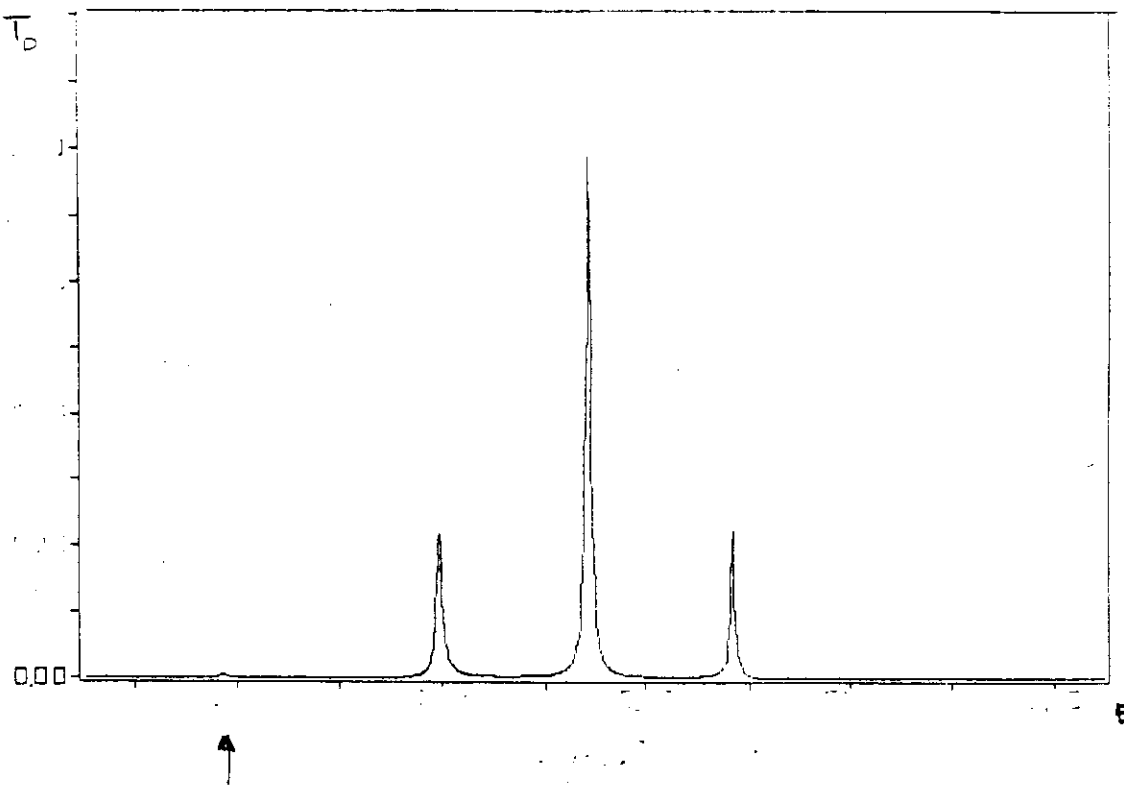
Symmetric structure



$V_0 = .25$

$m^* = .08\, m_e$

Asymmetric structure



$V_1 = .205$ $V_4 = .268$

$V_2 = .214$ $V_5 = .250$

$V_3 = .231$

Coherent Tunneling Current

[Low T
[$eV > E_F$

$$I = \frac{e m^* k}{2\pi^2 \hbar^3} \int_0^{E_z} dE_z \, (E_F - E_z) T(E_z)$$

$$T(E_z) = \frac{\Gamma_n^0 \Gamma_n^L}{(E_z - \varepsilon_n)^2 + \Gamma_n^2/4} = T(\varepsilon_n) \frac{\Gamma_n^2/4}{(E_z - \varepsilon_n)^2 + \Gamma_n^2/4}$$

$$T(\varepsilon_n) = \frac{4 \Gamma_n^0 \Gamma_n^L}{\Gamma_n^2}.$$

- Sharp resonance $E_n >> \Gamma_n$

$$\frac{\Gamma_n^2/4}{(E_z - \varepsilon_n)^2 + \Gamma_n^2/4} \simeq \frac{\pi \Gamma_n}{2} \delta(E_z - \varepsilon_n)$$

$$I = \frac{e m^* k}{4\pi \hbar^3} (E_F - \varepsilon_n) \Gamma_n T(\varepsilon_n)$$

$$\varepsilon_n \simeq \varepsilon_n^0 - \frac{eV}{2}$$

- good approximation.

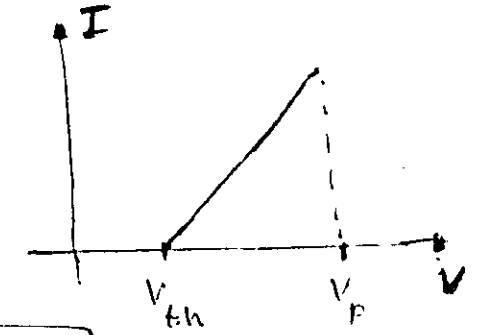
TIM * Esai: 1/7

ε_n^0 resonance energy at zero bias voltage.

- Total and partial decay widths are modified by the applied voltage and consequently, $T(\varepsilon_n)$.

$$I = \frac{e m^*}{4\pi \hbar^3} \left(E_F - \varepsilon_n^0 + \frac{eV}{2} \right) \Gamma_n T(\varepsilon_n)$$

$$\begin{cases} eV_{th} = 2(\varepsilon_n^0 - E_F) \\ eV_p = 2\varepsilon_n^0 \end{cases}$$



$$I_p = \frac{e m^*}{4\pi \hbar^3} E_F \Gamma_n T(\varepsilon_n)$$

peak resonant contribution

Time scale for coherent tunneling

For decay processes:

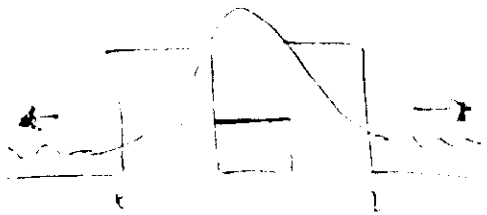
$$|\psi_n(x,t)|^2 = |\psi_n(x)|^2 \, e^{-\Gamma_n t/\hbar}$$

$$\boxed{\tau \sim \frac{\hbar}{\Gamma_n}}$$ lifetime

- intrinsic property of the system

For scattering one finds related notions involving Γ_n.

Notes: Re distinction on which channel dominates the decay rate.



Inelastic effects.

- Specific mechanisms
  - electron-phonon interaction
  - scattering by impurities
  - electron-electron interactions, etc.

- Phenomenological approach $V = V_0 - i\Gamma W$

Borrowed from Nuclear Physics;

Main effect of W is to absorb part of the incident flux. i.e. a new channel is introduced.

Schrodinger eq.

$$\boxed{\psi_n''(z) + \left[k_n^2 - V_0(z) + i\Gamma W(z)\right]\psi_n(z) = 0}$$

boundary conditions

$$\frac{\psi_n'(0_+)}{\psi_n(0)} = -ik_n$$

$$\frac{\psi_n'(l_+)}{\psi_n(l_+)} = ik_n$$

notice $W(z) \to 0$ $\quad \psi_n(z) \to \psi_n(z)$

Equation of continuity:

$$\frac{\partial}{\partial t}\int_0^L |\psi_n(z,t)|^2 = J_n(0,t) - J_n(L,t) + \frac{i}{\hbar} P_n e^{-\Gamma_n t/\hbar}$$

where $P_n = \int_0^L |\psi_n(z)|^2 W(z)\, dz$, $\quad E_n = \varepsilon_n - i\frac{\Gamma_n}{2}$

Proceeding in a similar fashion as in the coherent case, i.e. using the boundary conditions for ψ_n's

$$\Gamma^t_n = (\gamma_n^0 + \gamma_n^L) + \Gamma_n^i$$

- $\gamma_n^0 = \hbar\left(\frac{\hbar k_n}{m}\right)\frac{|\psi_n(0)|^2}{\int_0^L |\psi_n(z)|^2 dz}$

- $\gamma_n^L = \hbar\left(\frac{\hbar k_n}{m}\right)\frac{|\psi_n(L)|^2}{\int_0^L |\psi_n(z)|^2 dz}$

- $\Gamma_n^i = 2\,\frac{\int_0^L |\psi_n(z)|^2 W(z)\, dz}{\int_0^L |\psi_n(z)|^2 dz}$

If $W(z) = W = \text{cte.}$

- $\boxed{\Gamma_n^i = 2W}$ (i, inelastic channel)

notice that there is no reason to expect

$$\begin{cases} \Gamma_n^0 = \gamma_n^0 \\ \Gamma_n^L = \gamma_n^L \end{cases}$$

- Transmission Coefficient.

$$T^e(E) = \frac{\gamma_n^0 \gamma_n^L}{(E-\varepsilon_n)^2 + (\Gamma_n^t)^2/4}$$

(e, elastic channel) coherent.

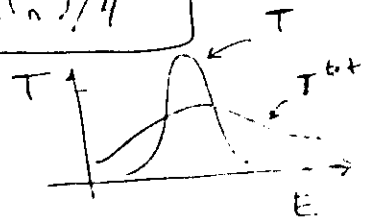
$$\boxed{T^e(E) = T_{res}\,\frac{(\Gamma_n^e/2)^2}{(E-\varepsilon_n)^2 + (\Gamma_n^t)^2/4}}$$

where $\boxed{\Gamma_n^e = \gamma_n^0 + \gamma_n^L}$; $T_{res} \equiv \frac{4\gamma_n^0\gamma_n^L}{(\Gamma_n^e)^2}$

$\boxed{\Gamma^t = \Gamma^e + \Gamma^i}$

Presence of new channel introduces an inelastic contribution to the transmission

$$T^{in} = T^{res}\,\frac{\Gamma_n^e\,\Gamma_n^i/4}{(E-\mathcal{E}_n)^2 + (\Gamma_n^t)^2/4}$$



$$T^t = T^e + T^i$$

$$T^t = T^{res}\,\frac{\Gamma_n^e\,\Gamma_n^t/4}{(E-\mathcal{E}_n)^2 + (\Gamma_n^t)^2/4}$$

e, elastic (coherent)
i, inelastic (incoherent)
t, total

notice $\dfrac{T^e}{T^i} = \dfrac{\Gamma_n^e}{\Gamma_n^i}$

Hence $\Gamma_n^e \gg \Gamma_n^i \Rightarrow T^e \gg T^i$

$\Gamma_n^e \ll \Gamma_n^i \Rightarrow T^e \ll T^i$

partial decay widths control which process dominant (inelastic)

Time and Scale Lecture

$$\begin{cases} \tau^e = \dfrac{\hbar}{\Gamma_n^e} \\ \tau^i = \dfrac{\hbar}{\Gamma_n^i} \end{cases}$$

Tunneling Current

- Sharp resonance $\mathcal{E}_n \gg \Gamma_n^t$

$$I^{tot} = \frac{e\,m^4}{2\pi^2\hbar^3}\int_0^{E_F}(E_F-E)\,T^t(E_z)\,dE_z$$

$$T^t(E_z) = T^{res}\,\frac{\Gamma_n^e}{\Gamma_n^t}\,\underbrace{\frac{(\Gamma_n^t)^2/4}{(E_z-\mathcal{E}_n)^2 + (\Gamma_n^t)^2/4}}_{\frac{\pi\,\Gamma_n^t}{2}\,\delta(E_z-\mathcal{E}_n)}$$

$$I^{tot} = \frac{e\,m^4}{4\pi\hbar^3}\,(E_F-\mathcal{E}_n)\,T^{res}\,\Gamma_n^e$$

does not depend on Γ_n^i !!

case analyzed [illegible]

i.e. For fully coherent structure ($\Gamma_n^i = 0$):

$$I = \frac{e m n^4}{4\pi \hbar^2} (E_F - \varepsilon_n)\, T(\varepsilon_n)\, \Gamma_n$$

For coherent plus incoherent case:

$$I^{tot} = \frac{e m n^4}{4\pi \hbar^2} (E_F - \varepsilon_n)\, T^{res}\, \Gamma_n^e$$

However:

$$T(\varepsilon_n) = \frac{4 \Gamma_n^0 \Gamma_n^L}{\Gamma_n^2} \quad ; \quad \Gamma_n = \Gamma_n^0 + \Gamma_n^L$$

and

$$T^{res} = \frac{4 \gamma_n^0 \gamma_n^L}{(\Gamma_n^e)^2} \quad ; \quad \Gamma_n^e = \gamma_n^0 + \gamma_n^L$$

assuming (Is this ok?)

$$\Gamma_n^0 = \gamma_n^0$$
$$\Gamma_n^L = \gamma_n^L$$

} same I-V characteristic !

- Tersoff & Grincwajg
  Appl. Phys. Lett. 52, 1739 (1987)
- Wolf & Winter
  Appl. Phys. Lett. 52, 1261 (1987)

$$I_{(coherent + incoherent)} = I_{(purely\ coherent)}$$

- In general both processes are present in resonant structures.
- Question: which one dominates? It is generally accepted that in systems with narrow barriers the process is mainly coherent and in systems with thick barriers, the incoherent contribution is the most important
- Stimulated emission

Dependence of resonant tunneling current on well width

Tsuchiya & Sakaki

Appl. Phys. Lett. 49, 88 (1986)

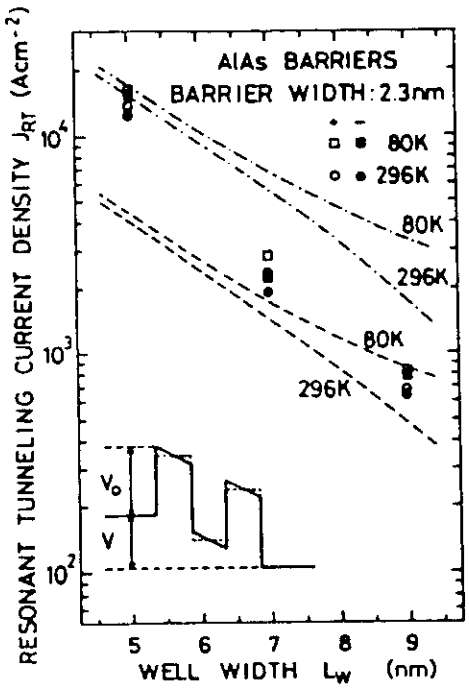


FIG. 3. Dependence of resonant tunneling current ($J_{RT} = J_p - J_v/2$) on well width L_w measured at 80 and 296 K. The theoretical curves are calculated after Ref. 1 using the square potential approximation (see the inset of the figure). The broken lines are obtained with Dingle's rule ($V_o = 1.355$ eV) and the dotted dash lines are for Miller's parameters ($V_o = 0.956$ eV).

ref. 1 Tsu & Esaki, Appl. Phys. Lett. 22, 562 (1973)

Dependence of resonant tunneling current on well width

Tsuchiya & Sakaki

Appl. Phys. Lett. 49, 88 (1986)

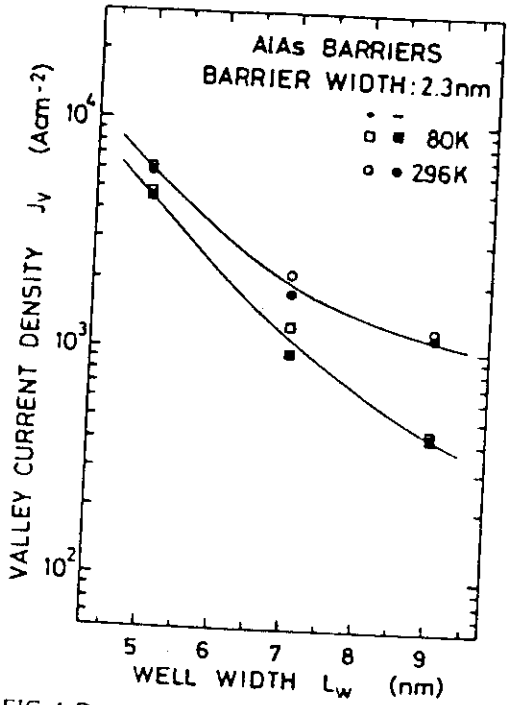


FIG. 4. Dependence of valley current J_v at 80 and 296 K on well width L_w.

Dependence of resonant tunneling current on Al mole fraction

Tsuchiya & Sakaki, Appl. Phys. Lett. 50, 1503 (1987)

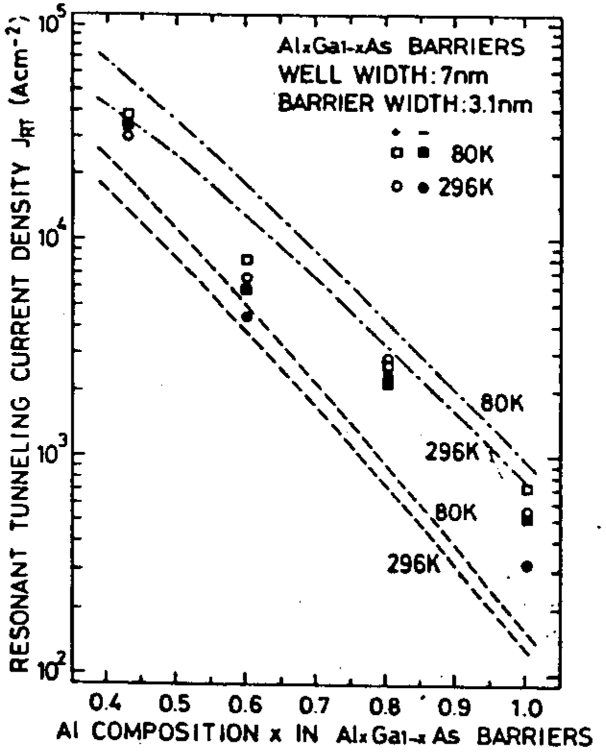
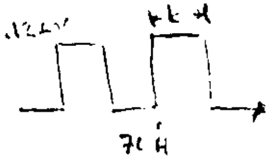


FIG. 3. Dependence of resonant tunneling current ($J_{RT} = J_p - J_V/2$) on x in the $Al_xGa_{1-x}As$ barrier measured at 80 and 296 K. The signs + and − indicate the polarity of bias voltage applied to the top electrode. The theoretical curves are calculated after Ref. 1 using the square potential approximation. The broken lines are obtained with Dingle's rule ($V_0 = 0.85\,\Delta E_g$) and the dot-dashed lines are for Miller's parameters ($V_0 = 0.6\Delta E_g$).

Peak currents as a function of barrier thickness

Guéret and co-workers

J. Appl. Phys. 66, 278 (1989)



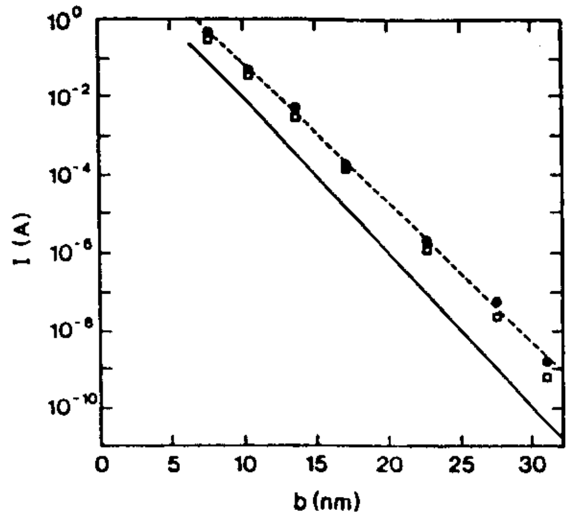


FIG. 4. Peak currents as a function of barrier thickness b. The values measured for positive and negative polarity are denoted by ● and □, respectively. The dashed line is according to Eq. (6). The solid line is the peak current calculated for the case of completely incoherent tunneling.

However: measured off resonance current levels are orders of magnitude more than from transmission formula.

($V<V_1$, $V>V_1$)

Theory vs experiment:

Sollner et al.
J. Appl. Phys. 63, 142 (1988)

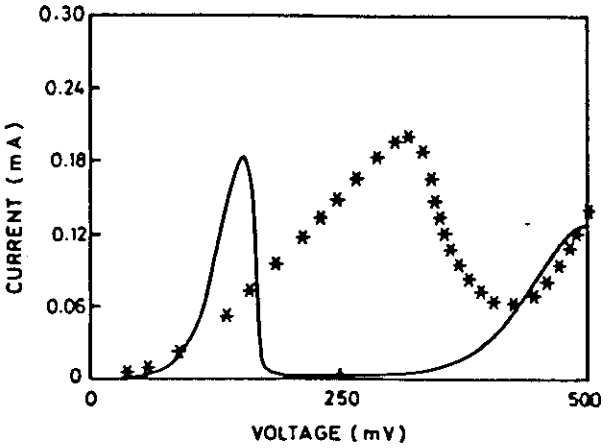


FIG. 3. A comparison of the experimental results of Sollner *et al.* (asterisks) with the numerical results (solid line) of Sec. II.

- Self consistent evaluation of the potential profile involving Sch. equation and Poisson eq.
  - Shinishi et al, Appl. Phys. Lett. 49, 1248 (1986)
  - Brennan, J. Appl. Phys. 62 3942 (1987)

- Experimental studies involving magnetic fields
  - Mendez, Esaki & Wang Phys. Rev. 33, 2893 (1986)
  - Goldman, Tsui & Cunningham Phys. Rev. 35, 9387 (1987)

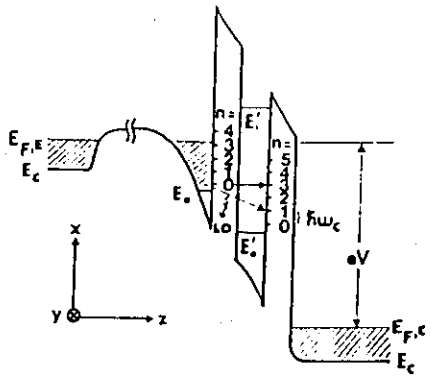


FIG. 3. The schematic conduction-band energy diagram of the device when biased in the valley current region, under magnetic field parallel to the z direction. Landau levels with indices from 0 to 5 are shown as short segments for both the source electrons and the metastable states in the quantum well. The arrow with a solid line indicates the elastic inter-Landau-level resonant tunneling ($\Delta n = 3$ is shown as an example), and the one with a dashed line indicates the phonon-emission-assisted resonant tunneling ($\Delta n = 2$, i.e., $2\hbar\omega_c = \hbar\omega_{LO}$).

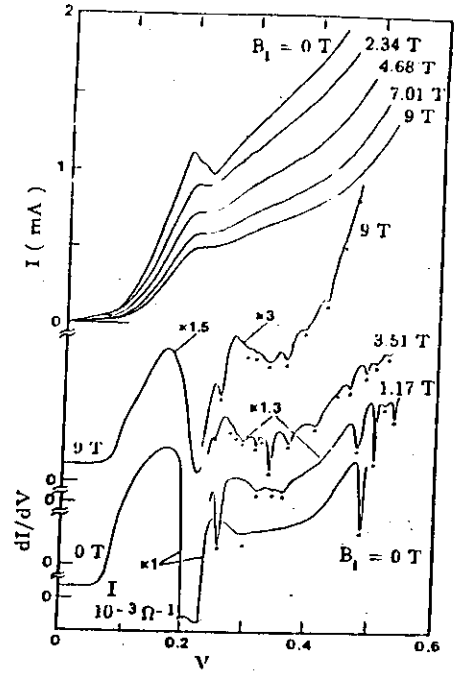


FIG. 1. I-V and G-V characteristics of the device under various magnetic fields at 4.2 K.

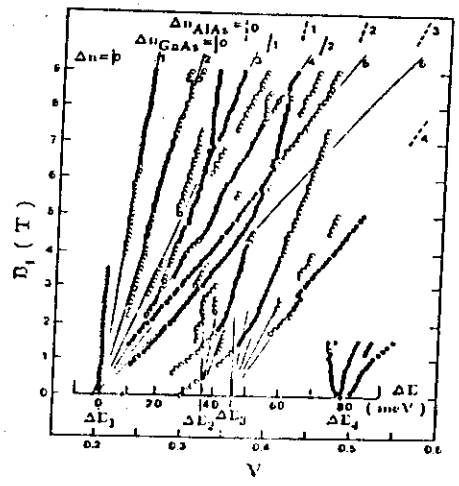


FIG. 2. The bias positions, at which the dips in the G-V curves are observed, are plotted as a function of $B_\parallel$. The ΔE scale is obtained experimentally, see context.

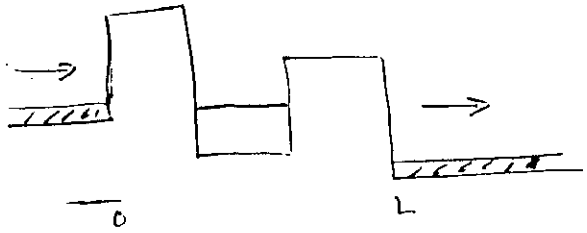
- work on specific inelastic mechanisms

  - electron-phonon interactions
  - electron-electron interactions
  - scattering by impurities in barriers and/or wells

  etc.

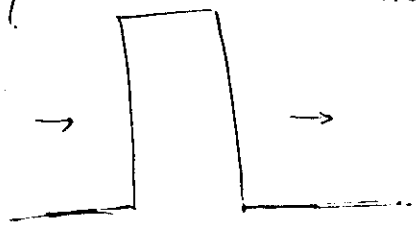
Tunneling times

main question: transit time through the structure



Theoretical controversy even for a single barrier

- no experiments!

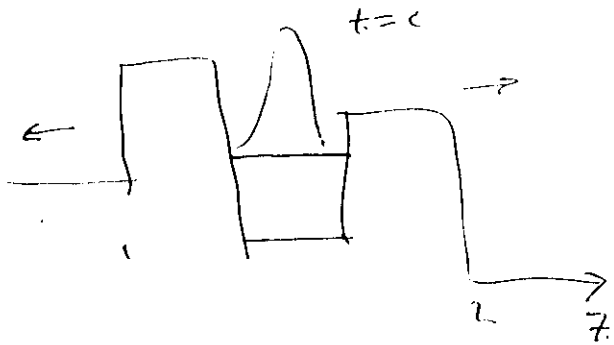


- Hauge, Rev. Mod. Phys. 61, 917 (1989)

Competing formalisms

- Dwell time
- Transmission phase time
- Traversal Larmor time

Decay or escape time



time evolution of initial state

$$H(t) = \int_0^L \phi(z,t)\,\phi(z,0)\,dz$$

$$P(t) = |H(t)|^2$$

$$\phi(z,t) = \int_0^L G^+(z,z';t)\,\phi(z',0)\,dz'$$

$$\rightarrow \boxed{\phi^+(z,z';t) = \int_C G^+(z,z';t)\,e^{-iEt/\hbar}\,dE}$$

$$G_1^+(z,z';t) = \frac{U_n(z)\,U_n(z')}{\hbar^2 k_n^2} + G(z,z';k)$$

$$P(t) = C_n \bar{C}_n e^{-\Gamma_n t/\hbar} + I \quad ; \quad \begin{cases} C_n = \int_0^L \phi\, U_n\,dz \\ \bar{C}_n = \int_0^L \phi^*\, U_n\,dz \end{cases}$$

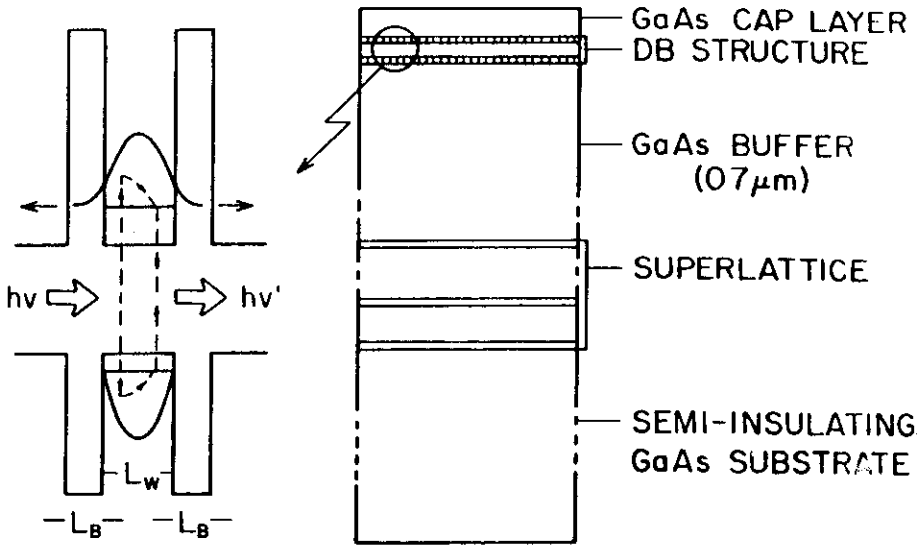
It is assumed: $C_n \bar{C}_n = 1$

$$\boxed{P(t) = e^{-\Gamma_n t/\hbar}}$$

Tunneling Escape

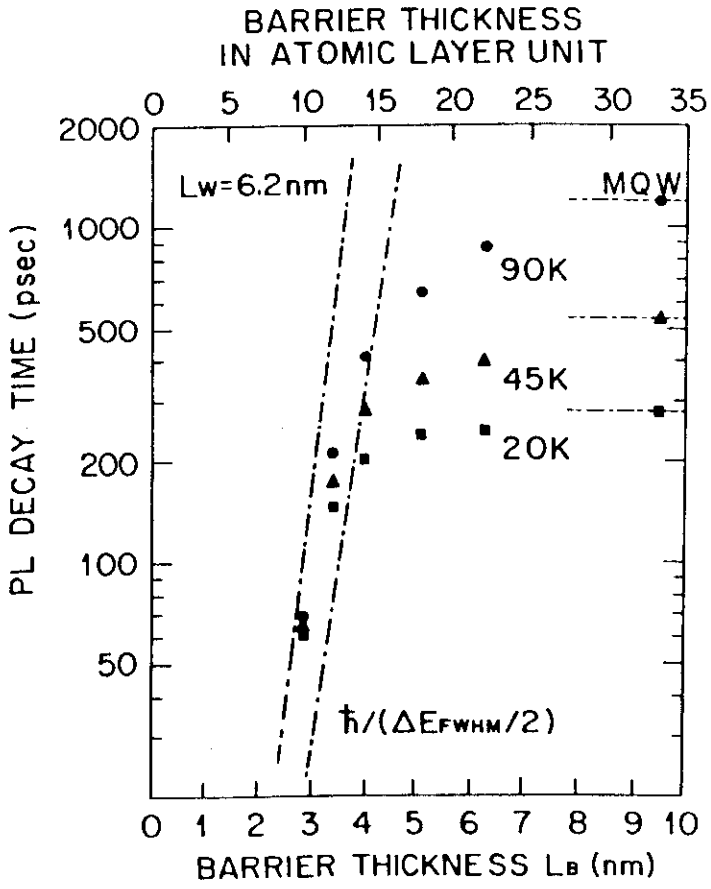
Tsuchiya, Matsuura & Sakaki

Phys. Rev. Lett. 59, 2356 (1987)



- radiative recombination process
- tunneling escape

Tsuchiya et al. (E2)



Jpn. J. Appl. Phys. 25, L871 (1986)

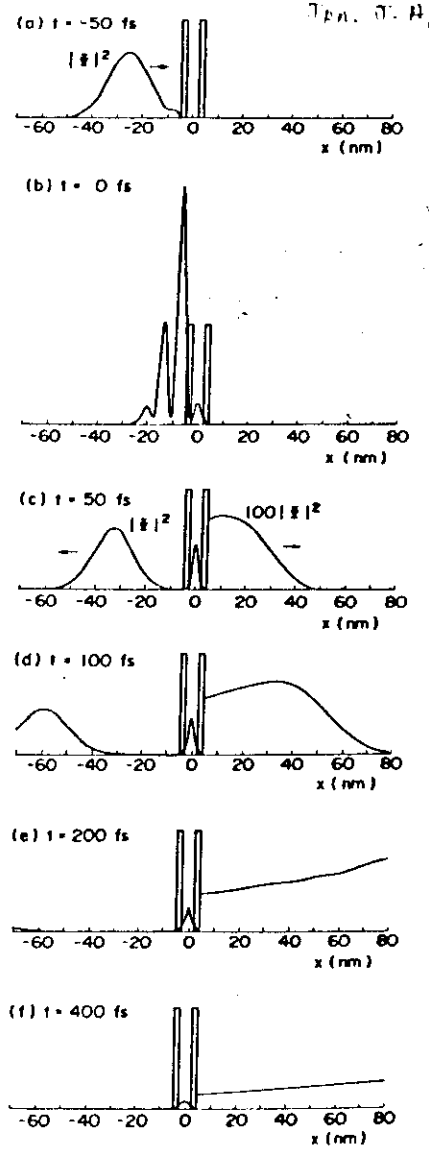


Fig. 1. Potential profile and the time evolution of an electron wave packet in a resonant tunneling system, where barrier height $V=400$ mV, barrier thickness $d=2$ nm, well width $L=5$ nm, average wave number of the incident wave packet $k_0=4.44\times10^9$ m^{-1} and wave number width $\Delta k=1\times10^9$ m^{-1}.

ponents, therefore there is a reflected wave. The wave packet in the well is in a quasi-stable resonant state and its amplitude decreases with time. Figure 3 shows how the amplitude of the wave packet in the well varies with

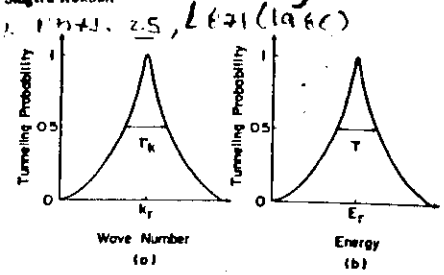


Fig. 2. Schematic illustrations of the tunneling probability as a function of wave number k and electron energy E. Definition of half widths Γ_k and Γ are also given.

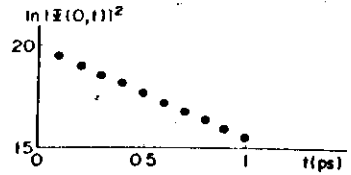


Fig. 3. Time dependence of amplitude of the wave packet shown in Fig. 1 at the center of the quantum well. Here, $|\psi|^2$ is not normalized.

Table I. Lifetime τ of the quantum well obtained from simulation of a wave packet.

V(mV)	L(nm)	d(nm)	τ(ns)
400	2	2	0.022
		4	0.37
		6	6.1
	5	2	0.23
		4	8.9
		6	360
	10	2	2.1
		4	110
		6	5900

V: barrier height, L: well width, d: barrier thickness.

time. It is seen that the amplitude decreases exponentially. We define the time-constant of the decay as the lifetime τ of the resonant state. Table I shows lifetime of resonant states under some device parametes. As barrier thickness increases or well width increases, the wave packet is trapped more tightly in the well and the lifetime becomes longer. Next, notice the transmitted wave packet. Since the wave packt tunnels out from the resonant state in the well, its width in k-space is Γ_k and is smaller than that of incident wave packet. The transmitted wave packet has well defined momentum (and energy) and its width in real space $\Delta x\equiv 1/\Gamma_k$ is large in comparison with the incident wave packet.

Here, we comment on the choice of the width Δk of the incident wave packet in k-space. Since width of energy distribution ΔE of a wave packet is given by

$$\Delta E=\hbar^2 k\Delta k/m, \tag{5}$$

the time width Δt of the incident wave packet becomes

• Dwell time (Smith, 60)

concept introduced by

G. Garcia-Calderon & A. Rubio
Solid State Commun. 41 (1982)

$$t_{DL} = \frac{m\kappa}{k}\int_0^L |\psi_I(E,x)|^2 dx = \frac{\kappa_n \Gamma_n^0}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}$$

I, incident from 0 < L

$$t_{LD} = \frac{m\kappa_n}{k}\int_0^L |\psi_r(E,x)|^2 dx = \frac{\kappa_n \Gamma_n^L}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}$$

r, incident from 0 < L

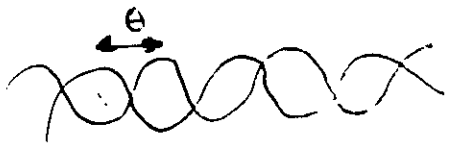
$$\boxed{t_{DL} = t_{LD}} \quad \text{if} \quad \Gamma_n^0 = \Gamma_n^L$$

- no adequate as a transit time except when $\Gamma_n^0 = \Gamma_n^L$ i.e., $T=1$.

If $\Gamma_n^L = 0 \Rightarrow T(\varepsilon_n) = 0$ no transmission

however $\boxed{t_{DL}(\varepsilon_n) = \frac{4\kappa_n}{\Gamma_n^0}}$

• Transmission Phase time



Eisenbud (48)

$t = |t| e^{i\theta}$

$$\boxed{\tau_\theta = \kappa \frac{d\theta}{dE}}$$

$\theta = \mathrm{Im}(\ln t)$; $\frac{d\theta}{dE} = \mathrm{Im}\left[\frac{1}{t}\frac{dt}{dE}\right]$

$t = \frac{(\Gamma_n^0 \Gamma_n^L)^{1/2}}{E - [\varepsilon_n - i\Gamma_n/2]}$

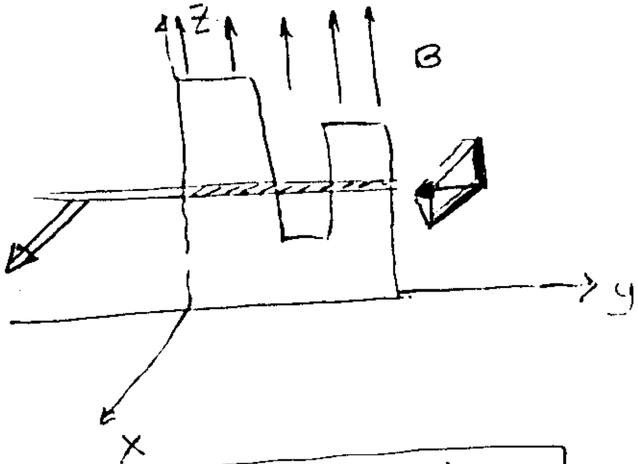
$$\boxed{\tau_\theta(E) = \frac{\kappa_n \Gamma_n/2}{(E-\varepsilon_n)^2 + \Gamma_n^2/4}}$$

$E = \varepsilon_n$; $\tau_r = \frac{2\kappa_n}{\Gamma}$

$\Gamma_n^a = \Gamma_n^L$; $\boxed{t_{DL} = t_{LD} = \tau_\theta = \frac{2\kappa_n}{\Gamma_n}}$

- <u>Traversal Larmor time</u>

Baz ('66), Rybachenko ('66), Büttiker ('83, '89)



$$\tau_T = \hbar \left[\left(\frac{\partial}{\partial V} \ln |t| \right)^2 + \left(\frac{\partial \theta}{\partial V} \right)^2 \right]^{1/2}$$

Variation with respect to the potential profile height V.

$$\frac{\partial}{\partial V} \ln |t| = C + \frac{(E - \mathcal{E}_n) \frac{\partial \mathcal{E}_n}{\partial V} - \frac{\Gamma_n}{4} \frac{\partial \Gamma_n}{\partial V}}{(E - \mathcal{E}_n)^2 + \Gamma_n^2/4} \ldots$$

$$C = \left[\frac{1}{\Gamma_n^1} \frac{\partial \Gamma_n^1}{\partial V} + \frac{1}{\Gamma_n^2} \frac{\partial \Gamma_n^2}{\partial V} \right] / 2$$

$$\frac{\partial}{\partial V} \theta = -\frac{1}{2} \frac{(E - \mathcal{E}_n) \frac{\partial \Gamma_n}{\partial V} + \Gamma_n \frac{\partial \mathcal{E}_n}{\partial V}}{(E - \mathcal{E}_n)^2 + \Gamma_n^2/4} \ldots$$

Typical Parameters

$V = .23$ eV

$w = b_1 = b_2 = 50$ Å

$m = .8\, m_e$

Voltage $= .1$ eV

<u>Complex eigenvalues and widths</u>

$\mathcal{E}_n = .12\,52\,30\,45\,01\,198$ eV

$\Gamma_n = .0000\,38\,308\,889$ eV

$\Gamma_n^1 = .0000\,7230\,1995$ eV

$\Gamma_n^2 = .000\,28\,00\,01\,8130$ eV

$\Lambda \approx 10^{-6} - 10^{-8}$

$\frac{\partial \mathcal{E}_n}{\partial V} = 1.00\,57$	$\frac{\partial \Gamma_n}{\partial V} = .000129$
$\frac{\partial \Gamma_n^2}{\partial V} = .00002\,3$	$\frac{\partial \Gamma_n^1}{\partial V} = .000\,130$

expression simplifies: $\Gamma_n = \Gamma_n^1 + \Gamma_n^2$

$$\tau_T = \frac{\hbar}{\left[(E-\epsilon_n)^2 + \Gamma_n^2/4\right]^{1/2}}$$

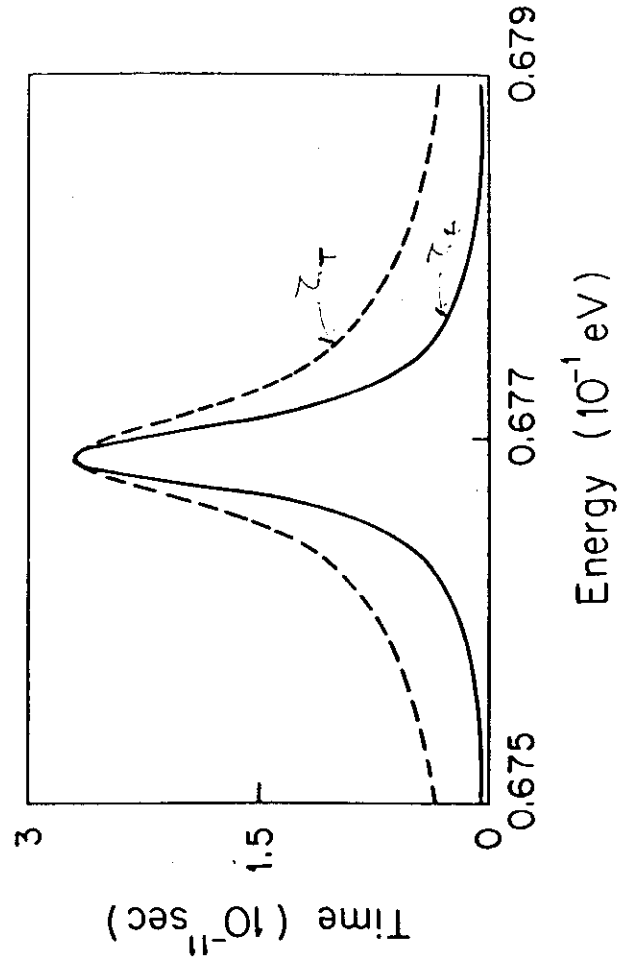
considered by

$\Gamma_n^1 = \Gamma_n^2$; Bethe (1939)

using a Wien argument

compared with:

$$t_b = \frac{\hbar\,\Gamma_n/2}{(E-\epsilon_n)^2 + \Gamma_n^2/4}$$



Example:

Conclusion: Phase [illegible]

[illegible] and [illegible]

[illegible] yield very similar results

close to resonance energies

i.e. they do not exaggerate

[illegible] results in this case.

Notice: contribution of resonance

i.e. $\Gamma_\epsilon = \Gamma_T = \frac{2\pi}{\Gamma}$ [illegible] the

a specific single energy. The physical

situation in semiconductor scattering

standards is different i.e. most

electrons participate almost [illegible]

in the [illegible] study.

Er

[illegible]

[illegible]

BACKGROUND MATERIAL

2 A 2: 2 C

Nuclear Physics A265 (1976) 443 – 460, © North-Holland Publishing Co., Amsterdam

RESONANT STATES AND THEIR USES

GASTÓN GARCÍA-CALDERÓN † and RUDOLF PEIERLS

Department of Theoretical Physics, 12, Parks Road, Oxford, England

Received 29 December 1975
(Revised 29 March 1976)

Abstract: The paper shows, for a simple model, how the wave functions belonging to complex energy eigenvalues (resonance states) can be regarded as part of a complete set of states, containing also bound states and a continuum of (generally complex) wave functions. This forms the basis of an expansion, which is used to describe inelastic scattering in the plane-wave Born approximation, taking the same simple model for the target.

1. Introduction

In recent years there has been increasing interest in the theoretical description of reactions leading to resonant, or decaying, states. In dealing with such, in principle unbound, final states, some authors have made use of scattering states [1]; others have used the complex states defined by Weinberg [2]. In this paper we shall use a description based on a physical definition of resonance states.

Resonance states were first used by Gamow [3]) in his work on α-decay. They are sometimes called Gamow states.

To describe such states we consider solutions of the Schrödinger equation which, at large distances, consist of purely outgoing waves. In other words, we require wave functions which do not contain any incoming components at infinite distance. This condition excludes stationary states, with real positive energies, but there exist complex energy eigenvalues, corresponding to states for which the density at each point in space decays exponentially in time.

The amplitude of such a wave function increases exponentially in space (representing the presence, at large distances, of particles emitted earlier from a stronger source) and therefore the usual rules concerning normalization, orthogonality and completeness of the eigenfunctions do not apply. For these reasons it was generally believed that the eigenfunctions belonging to resonant states were not very useful tools for calculation.

In the last decade the properties of such functions have been studied, and an important step has been the formulation of a useful rule for their normalization. Various approaches have led to the same normalization convention. Zel'dovich [4])

† Present address: Instituto de Física, Universidad Nacional Autónoma de México, México 20, DF.

first used an argument based on analytic continuation. His rule was adopted by Berggren [5]. We prefer a derivation starting from the behaviour of the Green function of the problem near its poles (which include the resonant states). The normalization rule so obtained is physically satisfactory in that it extends the validity of the standard result of first-order perturbation theory for a change in the internal potential of the system, by which the change in the energy eigenvalue is expressed as the integral of the perturbing potential times the square of the wave function. This point was made by Hokkyo [6]. We shall consider the derivation of the normalization of resonant states in sect. 2.

Using the relation of resonant states with the poles of the constant-energy Green function, one can derive expressions for the time-dependent Green function, in which resonant states enter in a very similar manner to bound states. Sect. 3 will discuss this representation, and show that there is some freedom in dividing the contribution between discrete resonance terms and a residual continuous spectrum. The limitations of this freedom of choice will also be discussed.

Sect. 4 contains a discussion of a simple model of inelastic scattering, including events which leave the target nucleus in a resonant state. For simplicity this is done in the framework of plane-wave Born approximation.

This approach has some similarity to that of Berggren [7]. It differs from his both in the arguments used and in the results. We do not propose to criticize his method in particular, but we found it difficult to convince ourselves of the validity of his arguments. For instance we found it hard to see how to interpret a Dirac δ-function of complex argument.

2. Normalization condition for complex energies

In this section we introduce the definition of resonant states and discuss the normalization condition for complex energies. For the sake of simplicity we shall initially restrict ourselves to the case of a particle of zero angular momentum in a static potential. The extension to higher angular momentum is straightforward, and we shall just state the results.

We then have to consider the radial Schrödinger equation

$$u''(r)+[k^2-V(r)]u(r)=0. \tag{2.1}$$

We have chosen units in which $\hbar = 2m = 1$; the energy is $E = k^2$ where k is the wave vector.

We assume the potential $V(r)$ to be of finite range i.e.

$$V(r)=0, \qquad r \geq R. \tag{2.2}$$

At the origin the radial wave function must vanish,

$$u(0)=0 \tag{2.3}$$

At large distances, $r > R$, the general solution of (2.1) is

$$u(r)=Ae^{ikr}+Be^{-ikr}. \tag{2.4}$$

Here the A-term represents a radially outgoing, the B-term a radially incoming wave [8]. The decaying state represents a situation in which there are no particles incident, and therefore $B = 0$, which corresponds to the condition

$$\frac{du(r)}{dr}-iku(r)=0; \qquad r \geq R. \tag{2.5}$$

We shall label the eigenvalues of k for which (2.1) has a solution satisfying boundary condition (2.5) by k_n and the wave functions by $u_n(r)$. Since, for real k, the relation $A(k) = B^*(k)$ holds, it becomes evident that we cannot satisfy the wave equation (2.1) with the boundary condition (2.5) for any real k_n. One easily verifies by using Green's formula between eq. (2.1) and its complex conjugate together with its respective boundary conditions that, for $\mathrm{Re}\, k_n \neq 0$,

$$\mathrm{Im}\, k_n = -|u_n(R)|^2 \int_0^R |u_n(r)|^2 dr. \tag{2.6}$$

If we choose the real part of k_n positive, which is consistent with our interpretation of the two terms of (2.4) as outgoing and incoming, repectively, the energy k_n^2 has a negative imaginary part, corresponding to an exponential decrease of the modulus of the wave function with time, as expected. For such states we write

$$k_n=\alpha_n-i\beta_n,$$

with positive β_n.

A negative imaginary part of k_n means also that the radial dependence of the wave function increases exponentially with distance. This property of the eigenfunction for decaying states has often led people to reject them as physically unreasonable. Yet this increase is entirely reasonable, because it reflects the fact that we are assuming an exponentially decaying state, and thus we see at distance r the particles emitted by the system a time r/v earlier, where v is their velocity, and these are more numerous by a factor $\exp(r/v\tau)$; τ being the mean life.

The above considerations mean that the usual methods of normalization and eigenfunction expansions are not valid for resonant states. This is not surprising because resonant states do not represent physical states of the system. In any real physical situation decaying states cannot have existed forever, but must have been created by some other physical process in the past. Nevertheless the pure decaying state is a convenient idealization if we are not interested in how it was obtained, just as it is convenient to use plane waves, which also cannot be normalized, when we are not interested in the practical limitations to our knowledge of the momentum.

[8] This interpretation is literally applicable if the real part of k is positive, but it is convenient for formal purposes to allow both signs.

A convenient way to connect resonant states with processes of physical interest is via the Green function of the Schrödinger equation with an outgoing boundary condition.

In what follows we study the behaviour of the Green function near one of its complex poles. We shall show that the residue of the Green function at the pole k_n is proportional to the functions $u_n(r)$ and $u_n(r')$, and that a convenient normalization condition for states of complex energy can be obtained by requiring the factor of proportionality to be the same as in the case of stationary states.

The Green function of eq. (2.1) satisfies the equation

$$\frac{\partial^2 G(r, r'; k)}{\partial r^2} + [k^2 - V(r)]G(r, r'; k) = \delta(r - r'), \tag{2.7}$$

with the boundary conditions at $r = 0$ and $r = R$ given respectively by

$$G(0, r'; k) = 0, \tag{2.8}$$

$$\left[\frac{\partial G(r, r'; k)}{\partial r} - ikG(r, r'; k)\right]_{r=R} = 0. \tag{2.9}$$

Near a complex pole $E_n = k_n^2$ the behaviour of $G(r, r'; k)$ can be expressed as

$$G(r, r'; k) = \frac{C_n(r, r')}{k^2 - k_n^2} + \chi(r, r'; k), \tag{2.10}$$

where $C_n(r, r')$ is the residue and $\chi(r, r'; k)$ is regular at k_n. Let us substitute (2.10) into (2.7). Rearranging terms the result may be written as

$$\frac{1}{k^2 - k_n^2}\left\{\frac{\partial^2 C_n(r, r')}{\partial r^2} + [k^2 - V(r)]C_n(r, r')\right\} + \left\{\frac{\partial^2 \chi(r, r'; k)}{\partial r^2} + [k^2 - V(r)]\chi(r, r'; k) - \delta(r - r')\right\} = 0. \tag{2.11}$$

Next we add and subtract in the above expression the quantity $k_n^2 C_n(r, r')/(k^2 - k_n^2)$ and take the limit as $k^2 \to k_n^2$. For consistency the terms containing $(k^2 - k_n^2)^{-1}$ and those having a constant limit as $k \to k_n$ must cancel separately:

$$\frac{\partial^2 C_n(r, r')}{\partial r^2} + [k_n^2 - V(r)]C_n(r, r') = 0, \tag{2.12}$$

$$\frac{\partial^2}{\partial r^2}\chi(r, r'; k_n) + [k_n^2 - V(r)]\chi(r, r'; k_n) + C_n(r, r') = \delta(r - r'). \tag{2.13}$$

It is now convenient to substitute (2.10) into the boundary conditions (2.8) and (2.9). We then proceed as in the previous case, and taking the limit $k^2 \to k_n^2$, we obtain,

$$C_n(0, r') = 0, \tag{2.14}$$

$$\chi(0, r'; k_n) = 0, \tag{2.15}$$

and also

$$\left[\frac{\partial}{\partial r} C_n(r, r') - ik_n C_n(r, r')\right]_{r=R} = 0, \tag{2.16}$$

$$\left[\frac{\partial}{\partial r}\chi(r, r'; k_n) - ik_n\chi(r, r'; k_n)\right]_{r=R} = \frac{i}{2k_n} C_n(R, r'). \tag{2.17}$$

We note that eq. (2.12) for $C_n(r, r')$ and its boundary conditions (2.14) and (2.16) are identical with eq. (2.1) for the function $u_n(r)$ and its boundary conditions, (2.3) and (2.5). Therefore the two functions must be proportional:

$$C_n(r, r') = u_n(r)P(r'). \tag{2.18}$$

In order to obtain an explicit expression for $P(r')$ we consider Green's formula between the equation for $u_n(r)$, (2.1), and that for $\chi(r, r'; k_n)$, (2.13). Integration from $r = 0$ to $r = R$ yields

$$[u_n(r)\chi'(r, r'; k_n) - \chi(r, r'; k_n)u_n'(r)]_0^R + \int_0^R u_n(r)C_n(r, r')dr = \int_0^R u_n(r)\delta(r - r')dr, \tag{2.19}$$

where the prime denotes the derivative with respect to the variable r. Using the corresponding boundary conditions (2.3), (2.5), (2.14), (2.17), and eq. (2.18), we finally have

$$P(r') = \frac{u_n(r')}{\int_0^R u_n^2(r)dr + (iu_n^2(R)/2k_n)}. \tag{2.20}$$

Therefore the residue of the Green function at the pole may be written as

$$C_n(r, r') = \frac{u_n(r)u_n(r')}{\int_0^R u_n^2(r)dr + (i/2k_n)u_n^2(R)}. \tag{2.21}$$

The appearance in (2.21) of the denominator suggests as a choice of normalization the condition

$$\int_0^R u_n^2(r)dr + \frac{i}{2k_n} u_n^2(R) = 1. \tag{2.22}$$

It is easy to verify from (2.1) and (2.5) that the appearance of R in this condition is spurious, and that the condition remains valid for any choice of R large enough to make the potential vanish. For bound states the limit $R \to \infty$ can be taken, and (2.22) then is the usual normalization rule.

The normalization condition (2.22) is equivalent to that suggested by Zel'dovich

using an argument based on analytic continuation. Choosing a normalization related to the residue at the pole of the Green function was suggested in the special case of the Lee model by Araki *et al.* [8]) and Goto [9]).

It is interesting to see that the normalization convention (2.22) has also a useful physical consequence in dealing with first-order perturbation theory. If one adds to the potential $V(r)$ a small perturbation $\delta V(r)$, which is assumed to vanish beyond R, then the change in the energy of a bound state is, to first order in $\delta V(r)$, by standard perturbation theory,

$$\delta k_n^2 = \int_0^R \delta V(r) u_n^2(r) \mathrm{d}r, \tag{2.23}$$

provided $u_n(r)$ is correctly normalized. With the convention (2.22) the first-order shift of a resonance level is given by the same expression. This is easily shown. Let us add to the potential of (2.1) a small perturbation, which is also assumed to vanish beyond R, then both the wave function $u_n(r)$ and the energy k_n^2 change by small amounts. The new function $\bar{u}_n(r)$ will therefore satisfy the equation

$$\bar{u}_n''(r) + [\bar{k}_n^2 - \bar{V}(r)]\bar{u}_n(r) = 0, \tag{2.24}$$

with the boundary conditions

$$\bar{u}_n(0) = 0, \tag{2.25}$$

$$\left[\frac{\mathrm{d}\bar{u}_n}{\mathrm{d}r} - i\bar{k}_n\bar{u}_n\right]_{r=R} = 0. \tag{2.26}$$

Using Green's formula between the equations for $u_n(r)$ and $\bar{u}_n(r)$ followed by integration from 0 to R, and the boundary conditions (2.3), (2.5), (2.25) and (2.26), we can write the result as

$$\delta k_n^2 = \bar{k}_n^2 - k_n^2 = \frac{\displaystyle\int_0^R u_n(r)[\bar{V}(r) - V(r)]\bar{u}_n(r)\mathrm{d}r}{\displaystyle\int_0^R \bar{u}_n(r)u_n(r)\mathrm{d}r + (i/k_n + \bar{k}_n)u_n(R)\bar{u}_n(R)} \tag{2.27}$$

Taking the limit $\bar{u}_n \to u_n$ and $\bar{k}_n \to k_n$, we find the change in energy to first order in $\delta V(r) = \bar{V}(r) - V(r)$. With the normalization convention (2.22) we obtain the same expression as in the case of a bound state, i.e. eq. (2.23). This result was noticed by Hokkyo [6]), who also expressed the normalization condition in the form (2.22).

For higher partial waves, analogous arguments lead to a boundary condition like (2.5), but with ik replaced by $kL_l(kR)$, where

$$L_l(kR) = \hat{h}_l'(kR)\,\hat{h}_l(kR) \tag{2.28}$$

is the logarithmic derivative of the Riccati-Hankel function, $\hat{h}_l(x) = h_l(x)\,x$, h_l being the spherical Hankel function. The normalization becomes

$$\int_0^R u_n^2(r)\mathrm{d}r + u_n^2(R)\left[\frac{\mathrm{d}}{\mathrm{d}k^2}(kL_l(kR))\right]_{k=k_n} \tag{2.29}$$

The same arguments can be used to derive the normalization condition for a many-body system, but its formulation is lengthy and will not be given here.

3. Time-dependent Green function

In the present section, we apply the result of the preceding section relating the resonant states with the poles of the energy-dependent Green function, to derive expressions for the retarded time-dependent Green function, in which resonant states enter in a very similar manner to bound states.

Since the retarded time-dependent Green function yields the solution of the initial-value problem for the time-dependent Schrödinger equation, we also discuss expansions of the time-dependent wave function in terms of bound and resonant states.

It is well known that the retarded Green function of the time-dependent wave equation, which serves to obtain the time evolution of the wave function, may be expressed as

$$g(r, r'; t) = \frac{\mathrm{i}}{2\pi}\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} G(r, r'; k)\mathrm{e}^{-\mathrm{i}Et}\mathrm{d}E, \tag{3.1}$$

where the integration in the E-plane passes above any singularities of $G(r, r'; k)$. In the present one-channel case, the discussion is simpler in the plane of momentum k. This is due to the fact that, as a function of energy, $G(r, r'; k)$ is no longer single-valued, because it has different values for k and $-k$, which belong to the same energy.

As in the previous section, we shall, for the sake of simplicity, restrict ourselves to the case of zero angular momentum. It follows then that $G(r, r'; t)$ satisfies eq. (2.7) and that $g(r, r'; k)$ obeys the one-dimensional equation

$$\left(i\frac{\partial}{\partial t} - H\right)g(r, r'; t) = i\delta(r - r')\delta(t), \tag{3.2}$$

where the Hamiltonian H is given by

$$H = -\frac{\partial^2}{\partial r^2} + V(r). \tag{3.3}$$

It is well known that for finite-range potentials [7] we may write the Green function

[7] Actually expression (3.4) remains valid for a more general class of potentials, namely those satisfying the conditions $\int_0^\infty |V(r)|\mathrm{d}r < \infty$ and $\int_0^\infty r|V(r)|\mathrm{d}r < \infty$.

$G(r, r'; k)$ as

$$G(r, r'; k) = -\phi(k, r_<) f(k, r_>) / J(k) \tag{3.4}$$

where $r_<$ indicates the smaller of r and r', and $r_>$ the larger. The function $\phi(k, r)$ is a regular solution of the time-independent Schrödinger equation (2.1) with boundary conditions at the origin $\phi(k, 0) = 0$ and $\phi'(k, 0) = 1$; the function $f(k, r)$ is irregular at the origin and is defined by the boundary condition:

$$f(k, r) = e^{ikr}, \qquad r > R,$$

finally, $J(k) \equiv f(k, 0)$ is the Jost function.

It is also well known that for finite-range potentials $G(r, r'; k)$ has an infinite number of poles corresponding to the zeros of the Jost function $J(k)$. These poles are, except in special cases, simple, and we shall assume that this is the case. They are distributed in the complex plane as shown in fig. 1. In general they lie either in the lower half of the k-plane or on the positive imaginary axis. The latter represent exponentially decreasing functions and belong to bound states; the former are associated with exponentially increasing functions, which are called anti-bound states when the poles are situated on the negative imaginary axis and resonant states otherwise. Actually, we shall be interested in a description involving resonant poles situated in the fourth quadrant of the complex k-plane such that Re $k_n > |\text{Im } k_n| > 0$. These poles for which Re $E_n > 0$, Im $E_n < 0$, are commonly called proper resonant poles.

In the momentum plane, the integration contour of eq. (3.1) becomes the contour c_0 shown in fig. 1. Since we are interested in the physics associated with the known poles, we are tempted to try to close the integration contour in the k-plane. However the factor $\exp(-ik^2t)$ diverges at large distances in the upper right and lower left quadrants, while it decreases rapidly, for reasonable t, in the other two directions. One can verify that the variation of $G(r, r'; k)$ with k is at most exponential. This follows by looking at the behaviour as $|k| \to \infty$ of the functions $\phi(k, r)$, $f(k, r)$ and $J(k)$ as studied by Newton [11], and then using eq. (3.4). Hence the behaviour of the integrand

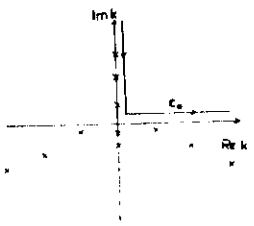


Fig. 1. Location of poles in k plane.

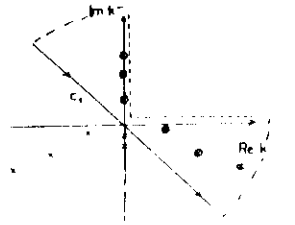


Fig. 2. Contour of steepest descent for time factor.

in (3.1) at large k is dominated by the factor $\exp(-ik^2t)$. As a result it is not possible to remove the whole contour to infinity, but we can deform it in the second and fourth quadrants. One useful choice is to deform the contour as shown schematically in fig. 2.

The straight line is the line of steepest descent of the factor $\exp(-ik^2t)$, and should lead to a moderately rapidly converging, and not too rapidly oscillating, integral for not too short times. By deforming the contour we have passed over some poles of $G(r, r'; k)$, including all those belonging to bound states, and the proper resonant states. We may now write the time-dependent Green function in the form

$$g(r, r'; t) = \sum_n u_n(r) u_n(r') e^{-iE_n t} + \frac{1}{\pi} \int_0^\infty \gamma z \, dz \, e^{-\gamma^2 z^2 t} G(r, r'; \gamma z). \tag{3.5}$$

Here the summation includes all bound states and all proper resonant states. In the integral contribution we have made the change of variable $k = \gamma z$, where z is a real variable and γ is an abbreviation for $\gamma = \sqrt{-i} = \sqrt{\frac{1}{2}}(1 - i)$. This simple representation of the time-dependent Green function was used by Scheffler [10].

It is convenient to combine, in the integral term of (3.5), the contributions from z and $-z$, so that the integral becomes

$$\frac{1}{\pi} \int_0^\infty \gamma z \, dz \, e^{-\gamma^2 z^2 t} [G(r, r'; \gamma z) - G(r, r'; -\gamma z)]. \tag{3.6}$$

The difference between the two Green functions in the bracket is, as a function of r, a solution of the homogeneous Schrödinger equation, as can be seen by subtracting (2.7) for opposite values of k. Thus the difference is proportional to $u(E, r)$, the solution of the Schrödinger equation for energy $E = -iz$, which vanishes at the origin. Because of the symmetry of the Green function, it is also proportional to $u(E, r')$. In order to write (3.5) as

$$g(r, r'; t) = \sum_n u_n(r) u_n(r') e^{-iE_n t} + \int_0^{-i\infty} dE \, u(E, r) u(E, r') e^{-iEt}, \tag{3.7}$$

we have to choose a suitable normalization for $u(E, r)$.

In order to have (3.6) take the form (3.7), we require that

$$\frac{i}{2\pi} [G(r, r'; k) - G(r, r'; -k)] = u(E, r) u(E, r'). \tag{3.8}$$

From the defining equation (2.7) and the Schrödinger equation for $u(E, r)$ one easily derives by cross multiplication and integration

$$u(E, R) G'(R, r'; k) - u'(E, R) G(R, r'; k) = u(E, r') \tag{3.9}$$

where the accents denote derivatives with respect to r. The same equation is also valid for $G(r, r'; -k)$. Using the boundary condition (2.9) for the Green functions, we find

$$G(R, r'; \pm k) = -\frac{u(E, r')}{u'(E, R) \mp iku(E, R)},$$

so that

$$G(R,r';k)-G(R,r';-k)=\frac{ku(E,R)u(E,r')}{\pi[u'(E,R)^2+k^2u(E,R)^2]} \tag{3.10}$$

The convention that will ensure (3.8) is therefore

$$u'(E,R)^2+k^2u(E,R)^2=k/\pi. \tag{3.11}$$

The left-hand side of (3.11) is independent of distance beyond the range of the potential, so that the equation also holds for any radius greater than R. It is easily verified that for real positive energy (3.11) becomes the standard normalization (per unit energy) in the continuous spectrum.

For the lth partial wave, the same argument leads to the result

$$[u'(E,R)-k\,L_l(kR)u(E,R)][u'(E,R)-k\,L_l(-kR)u(E,R)]=\frac{k}{2\pi i}[L_l(kR)-L_l(-kR)], \tag{3.11a}$$

in place of (3.11). Here L_l is the logarithmic derivate of the Riccati-Hankel function, as in (2.28). It is again easy to verify that (3.11a) is independent of R, and that for real E it reduces to the conventional normalization in the continuous spectrum.

Let us now discuss the solution of the initial-value problem in which the wave function is given, at $t=0$, in terms of an expansion involving bound and Gamow states. We have

$$\psi(r,t)=\int_0^\infty g(r,r';t)\psi(r',0)\mathrm{d}r', \tag{3.12}$$

where $\psi(r,t)$ obeys the time-dependent Schrödinger equation

$$\left(i\frac{\partial}{\partial t}-H\right)\psi(r,t)=0, \tag{3.13}$$

and H is the Hamiltonian given by (3.3).

Substituting (3.7) into (3.12) we find

$$\psi(r,t)=\sum_n a_n u_n(r)e^{-iE_nt}+\int_0^{-i\infty}b(E)u(E,r)e^{-iEt}\mathrm{d}E, \tag{3.14}$$

where the coefficients a_n and $b(E)$ are given by

$$a_n=\int_0^\infty u_n(r)\psi(r,0)\mathrm{d}r, \tag{3.15}$$

$$b(E)=\int\mu(E,r)\psi(r,0)\mathrm{d}r. \tag{3.16}$$

If the initial wave function $\psi(r,0)$ vanishes beyond a certain range, then the integrals (3.15) and (3.16) involve only finite integration and raise no problems. If, however, the initial function decreases only exponentially, say as $\exp(-\alpha r)$, for large r, then the integrals diverge if the imaginary part of k_n, or $k=\gamma z$, respectively, is less than $-\alpha$. In that case we can deform the contour c_0 as shown in fig. 3. The new integration contour runs parallel to the real axis from some suitable points with imaginary parts $-\alpha$ and α. The summation in (3.14) then includes only poles above c_2.

It is convenient to observe that the normalization condition for continuum states of complex energy depends only on E, but not on the shape of the contour. In particular for $\alpha=0$, when the sum includes only bound states, and the integral

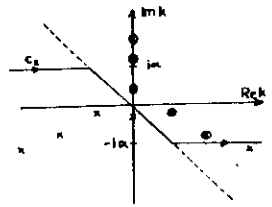


Fig. 3. Integration contour suitable when the wave function goes asymptotically as $\exp(-r)$.

extends over real positive energies, it is easily verified that the rule (3.11) for the normalization of $u(E,r)$ then reduces to the usual rule for normalization in the continuous spectrum.

It is interesting to observe that relation (3.14) can be applied at time $t=0^+$, and then amounts to expand a general function in terms of a sum over bound and resonant terms, and an integral over a continuum. That means we come close to treat resonant states as part of a complete set of eigenfunctions.

In this we should note some limitations: the completeness in terms of a specific contour applies only if we restrict the space of functions to be expanded to those decreasing fast enough at infinity. The most convenient contour, i.e. that of fig. 2, which presumably gives the most rapidly converging integral term, goes only with functions decreasing faster than any exponential. If we want to be able to expand any function decreasing exponentially we may use the contour of fig. 3. In the case of functions decreasing less than exponentially we take $\alpha\to 0$. This leaves us with the conventional representation in terms of bound states and a continuum over all real positive energies.

The other limitation is that the coefficients a_n and $b(E)$ cannot be interpreted as probability amplitudes, since the sum of their square moduli does not add up to the norm of the expanded function. This is related to the occurrence in all these equations of the square of an eigenfunction, not its square modulus.

Nevertheless Gamow states can be useful in dealing with practical problems, such as inelastic scattering of particles, resulting in an unbound state of the target. This is the subject of the next section.

4. Inelastic scattering

We consider a simple reaction model. We believe that it contains the essential qualitative features of more realistic models and that it is adequate to discuss the main characteristics of the idea of using Gamow states as final states in direct reactions.

We assume a "nucleus" consisting of one particle, coordinate r, in a potential $V(r)$ in the same units as above, initially in its ground state $\chi_0(r)$. The nucleus is hit by a projectile, radius vector ξ, which interacts only with the r-particle, by an interaction $w(r-\xi)$. Hence the system is described by the Schrödinger equation,

$$\left[i\frac{\partial}{\partial t} - H_r - T_\xi\right]\Phi(r,\xi,t) = w(r-\xi)\Phi(r,\xi,t), \tag{4.1}$$

where T_ξ is the kinetic energy of the projectile, which is assumed to have initial wave vector p_i, and H_r represents the nuclear Hamiltonian. If $w(r-\xi)$ is regarded as small, and its square neglected, this amounts to the first-order Born approximation. To first order we then have to solve the equation

$$\left[i\frac{\partial}{\partial t} - T_\xi - H_r\right]\Phi(r,\xi;t) = w(r-\xi)e^{i(p_i\cdot\xi}\chi_0(r)e^{-i(E_0+p_i^2)t}, \tag{4.2}$$

where E_0 is the ground-state energy of the nucleus.

We want to know the transition cross section for collisions in which the projectile is emitted with wave vector $p' = p_i + q$. Then we may project from (4.2) the Fourier component of wave vector p' in ξ. This is easily done by first forming the Fourier transform of $\Phi(r,\xi;t)$ with respect to the coordinates of the scattered particle, i.e.,

$$\Phi(r,\xi;t) = \int dp'' e^{ip''\cdot\xi}e^{-ip''^2t}\psi_{p''}(r,t), \tag{4.3}$$

where $\psi_{p''}(r,t)$ represents the wave function of the nucleus. Then we substitute the above expression into (4.2) followed by multiplication by $(1/(2\pi)^3)/\exp(-ip_i\cdot\xi)$, and integration through space. We are left with an equation for $\psi_{p'}(r,t)$, namely,

$$\left[i\frac{\partial}{\partial t} - H_r\right]\psi_{p'}(r,t) = w(q)e^{iq\cdot r}\chi_0(r)e^{-i\varepsilon' t} = F_q(r)e^{-i\varepsilon' t} = F_q(r,t), \tag{4.4}$$

where $\varepsilon' = E_0 + p_i^2 - p'^2$ is the final energy of the nucleus, and $w(q)$ is the Fourier transform of the potential $w(r-\xi)$ with respect to the ξ-coordinates.

We denote the right-hand side of (4.4), which acts as the "source" in our inhomogeneous equation, by $F_q(r,t)$. The left-hand side of (4.4) is the time-dependent equation for a Hamiltonian of the same type as that discussed in the previous section. The most obvious suggestion would be to use the time-dependent Green function, $g(r,r';t)$, to solve (4.4) for $\psi_{p'}(r,t)$ and then find the norm of the latter. However, the transition probability $I_{p'}(t)$ to all states in which the projectile ends up with wave vector p', which is the quantity of interest, is given by the norm of $\psi_{p'}(r,t)$, i.e.

$$I_{p'}(t) = \int dr\psi^*_{p'}(r,t)\psi_{p'}(r,t). \tag{4.5}$$

This would require computing the space integral of the square modulus of an expression of a form similar to (3.14) and would be very impractical. Instead we notice that, by the usual continuity arguments, one can derive from (4.4) the relation,

$$\frac{\partial}{\partial t}\int dr\psi^*_{p'}(r,t)\psi_{p'}(r,t) = \frac{1}{i}\int dr[\psi^*_{p'}H\psi_{p'} - \psi_{p'}(H\psi_{p'})^*] + \frac{1}{i}\int dr[\psi^*_{p'}F_q - \psi_{p'}F^*_q]. \tag{4.6}$$

Since $H = H^*$ it follows, by using Green's theorem, that the first term on the right-hand side of (4.6) vanishes. Consequently, the transition probability, at time t after the beginning of the collision is,

$$I_{p'}(t) = \frac{1}{i}\int_0^t dt'\int dr[\psi^*_{p'}(r,t')F_q(r,t') - \psi_{p'}(r,t')F^*_q(r,t')] \tag{4.7}$$

This is now a linear relation in $\psi_{p'}(r,t)$. Since our quantities depend on vectors, in order to use the ideas presented in the preceding section, one should consider an angular momentum representation of relation (4.7). However, it is more convenient to continue the analysis in the present form and work out the angular momentum representation afterwards. Therefore we note that, in the present situation, the Green function associated with $\psi_{p'}(r,t)$ obeys the equation,

$$\left[i\frac{\partial}{\partial t} - H_r\right]g(r,r';t-t') = i\delta(r-r')\delta(t-t'). \tag{4.8}$$

We impose the causality condition

$$g(r,r';t-t') = 0, \qquad t < t'. \tag{4.9}$$

Consequently we may write the solution of (4.4) as

$$\psi_{p'}(r,t) = \frac{1}{i}\int dr'\int_0^t dt' g(r,r';t-t')F_q(r')e^{-i\varepsilon' t'}. \tag{4.10}$$

Using the Fourier transform of g, as in (3.1), we obtain an expression in which the time integration over t' can be performed without difficulty. Hence

$$\psi_{p'}(r,t) = \frac{i}{2\pi}\int dr'\int_{-\infty} dk G(r,r',k)F_q(r')e^{-i\varepsilon' t'}\frac{e^{-i(k-\varepsilon')t}-1}{k-\varepsilon'}. \tag{4.11}$$

where $\Delta = \varepsilon' - E$ and $E = k^2$. Using this result in (4.7) we obtain a result for the transition probability which can be further simplified by performing the remaining time integration. If we define the quantity $h_E(t)$ by

$$h_E(t) = i\int_0^t \mathrm{d}t' \frac{1-\mathrm{e}^{i\Delta t'}}{\Delta} = \frac{it}{\Delta} - \frac{\mathrm{e}^{i\Delta t}-1}{\Delta^2}, \tag{4.12}$$

the transition probability may be written as

$$I_{p'}(t) = -\frac{1}{\pi}|w(q)|^2 \operatorname{Im}\left\{\int \mathrm{d}r\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}}\chi_0^*(r)\int \mathrm{d}r'\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}'}\chi_0(r)\int_{c_0}\mathrm{d}E G(r,r',k)h_E(t)\right\}. \tag{4.13}$$

It is now convenient to expand the expression in curly brackets in terms of spherical harmonics. We assume for simplicity that the ground-state wave function has zero angular momentum and is real. The transition probability becomes

$$I_{p'}(t) = \sum_l I_{p'l}(t), \tag{4.14}$$

where $I_{p'l}(t)$, the transition probability to a final angular momentum l, is

$$I_{p'l}(t) = -\frac{1}{\pi}|w(q)|^2(2l+1)\int \mathrm{d}r j_l(qr)u_0(r)\int \mathrm{d}r' j_l(qr')u_0(r')\operatorname{Im}\int_{c_0}\mathrm{d}E G_l(r,r';k)h_E(t). \tag{4.15}$$

Here $j_l(qr)$, $u_0(r)$ and $G_l(r,r';k)$ are, respectively, the lth spherical Bessel function, the radial ground-state wave function, and the l-wave radial Green function.

We may evaluate the energy integral in (4.15) by a suitable deformation of the contour. In the present case the most convenient contour is the one shown in fig. 3. The purpose of this choice, as discussed in sect. 3, is to avoid divergent radial integrals. The partial transition probability now becomes

$$I_{p'l}(t) = 2|w(q)|^2(2l+1)\operatorname{Re}\left\{\sum_b F_{lb}^2(q)h_{E_b}(t) + \sum_r F_{lr}^2(q)h_{E_r}(t) + \int_{c_2}\mathrm{d}E F_{lk}^2(q)h_E(t)\right\}, \tag{4.16}$$

where the subscripts b and r stand, respectively, for bound and resonant states, and the wave vector k lies on the contour c_2. The quantities $F_{ln}(q)$ with $n = b$ or r, and F_{lk} are the matrix elements

$$F_{ln}(q) = \int_0^\infty j_l(qr)u_0(r)u_n(r)\mathrm{d}r, \tag{4.17}$$

$$F_{lk}(q) = \int j_l(qr)u_0(r)u(E,r)\mathrm{d}r. \tag{4.18}$$

Similarly the time factors $h_{E_n}(t)$ and $h_E(t)$ are

$$h_{E_n}(t) = \frac{it}{\Delta_n} - \frac{\mathrm{e}^{i\Delta_n t}-1}{\Delta_n^2}, \tag{4.19}$$

$$h_E(t) = \frac{it}{\Delta_E} - \frac{\mathrm{e}^{i\Delta_E t}-1}{\Delta_E^2}, \tag{4.20}$$

where, of course, $\Delta_n = \varepsilon' - E_n$ and $\Delta_E = \varepsilon' - E$. For bound states E_n is real. However, for resonant states $E_r = \varepsilon_r - \frac{1}{2}i\Gamma_r$ is a complex quantity, as are the values of E on c_2.

From the expression (4.14) for the transition probability we can obtain the energy distribution for the residual "nucleus", by considering times long compared to the natural periods of the system. For bound states, for which F_{lb} is real, the time factors reduce to

$$2(1-\cos\Delta_b t)/\Delta_b^2 \approx 2\pi t\delta(\Delta_b),$$

which is manifestly linear in t. For complex argument, on the other hand, the exponential terms in the time factors (4.19) and (4.20) are small, and the leading term is again proportional to t. The differential cross section is

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega_{p'}\mathrm{d}E'} = \frac{1}{4(2\pi)^3}\frac{p'}{p_i}\sum_l \omega_{p'l}, \tag{4.21}$$

where $E' = p'^2$ is the energy of the scattered particle, and $\omega_{k'l}$ is the transition probability per unit time to a state of angular momentum l:

$$\omega_{p'l} = \frac{1}{t}I_{p'l}(t) = |w(q)|^2(2l+1)\left\{2\pi\sum_b F_{lb}^2\delta(E'-E_b) + \sum_r \frac{i(F_{lr}^2 - F_{lr}^{*2})(\varepsilon'-\varepsilon_r) + \frac{1}{2}\Gamma_r(F_{lr}^2 + F_{lr}^{*2})}{(\varepsilon'-\varepsilon_r)^2 + \frac{1}{4}\Gamma_r^2} + \operatorname{Re}\left[i\int_{c_2}\mathrm{d}E F_{lk}^2/\Delta_E\right]\right\}. \tag{4.22}$$

It is convenient to introduce the real and imaginary parts of the complex matrix element F_{lr}

$$F_{lr}(q) = x_{lr}(q) - iy_{lr}(q). \tag{4.23}$$

We may then write (4.22) in a slightly more transparent form:

$$\omega_{p'l} = \frac{1}{t}I_{p'l}(t) = |w(q)|^2(2l+1)\left\{2\pi\sum_b F_{lb}^2\delta(\varepsilon'-E_b) + \sum_r \frac{4x_{lr}y_{lr}(\varepsilon'-\varepsilon_r) + 2\Gamma_r(x_{lr}^2 - y_{lr}^2)}{(\varepsilon'-\varepsilon_r)^2 + \frac{1}{4}\Gamma_r^2} - \operatorname{Im}\int_{c_2}\mathrm{d}E\frac{F_{lk}^2}{\Delta_E}\right\}. \tag{4.24}$$

We observe that bound and resonant states contribute clearly defined terms, each peaked at an energy corresponding to an excited state of the "nucleus". The integral term, as well as the distant terms in the sum, contribute a background which is, in principle, well defined, and which will vary slowly with energy. The contribution of each resonant term to the differential cross section is real, but not necessarily

positive. However, if a level is narrow, compared to its distance from the adjacent resonances, its wave function is predominantly real, and its contribution positive. If the levels overlap there is no reason why some contributions should not become negative, as long as the total remains positive.

5. Discussion and extensions

The main result of sect. 4 is that, for a moderately narrow resonant state, the transition probability can be computed exactly as for a bound state, using in the integral for the matrix element the wave function with the normalization convention (2.22) or (2.29). This result has been obtained for the very primitive model of sect. 4, and in first-order plane-wave Born approximation.

The extension to distorted-wave Born approximation is straightforward. The main further complication is that the right-hand side of (4.4) becomes less simple, and depends no longer just on the momentum transfer, but separately on the initial and final momentum of the projectile.

For real nuclei, containing more than one nucleon, the normalization rule (2.29) can be generalized. The first term becomes an integral over the "internal" configuration space, i.e. the region in which no nucleon is further than R from the centre. This region is bounded by many channels; each corresponding to the escape beyond R of a nucleon of given angular momentum and spin, leaving the residual nucleus in a given state. The second term of (2.29) now becomes a sum over channels, each having one nucleon at distance R and involving an integration over all remaining variables. Difficulties arise, as usual, with channels involving the escape of two or more nucleons, since their interactions are not necessarily negligible when they are beyond R.

The Green function now becomes many-valued, with a square-root type branch point, as a function of the energy, at the threshold energy for each channel.

Contour integration similar to that in sect. 3 now leaves a continuous-spectrum type integral starting from each of these branch points. As in sect. 3 it is convenient to avoid violent oscillations in the integrals by following the line of constant phase of the dominant factor $\exp(-iEt)$. This line is a vertical in the energy plane.

In fig. 4, c_1 shows the cut in the energy plane which is the image of the k-plane contour c_1 of fig. 2b. Similar cuts $c_1', c_1'', \ldots$ start from the new branch points, and the generalization of (3.7) contains an integral along each of these cuts.

Swinging the cuts down from the positive real E-axis, which is their conventional position, opens up a number of poles (which, with the conventional choice of cut, would be on unphysical sheets of the Riemann surface), and they will contribute discrete decaying terms as in (3.7).

We have not investigated the distribution of poles which will appear explicitly with this choice of the cuts. It is plausible that they will include all long-lived resonances of physical interest, but this needs further discussion.

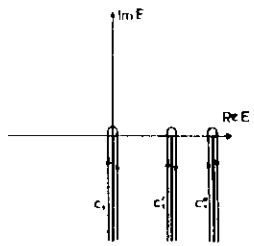


Fig. 4. Cuts and contours in energy plane for multi-channel problem.

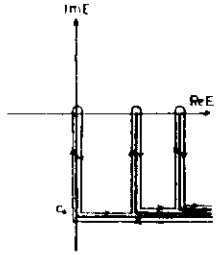


Fig. 5. As in fig. 4, but for wave functions with exponential tails in all channels.

If one requires the expansion of a function which decreases exponentially at large distances, one has to bridge the gaps between the cuts by lines limiting the imaginary parts of all channel momenta whose thresholds have been passed, so that the generalization of fig. 3 would, in the energy plane, look somewhat like fig. 5. If we wish to combine the contributions from the two sides of each cut, so as to maintain an expression of the form (3.7) the contour must reach and leave the cut at the same point, as in fig. 5. One simple way of achieving this is to choose the contour as a horizontal line in the energy plane.

We have not studied the general expression in detail, but it is clear that, as in sect. 4, the differential cross section for inelastic scattering will still consist of discrete contributions from the bound and long-lived resonant states, plus a continuous background, which may be expected to vary slowly with energy in the resonance region.

The discussion of this paper was based on finite-range interaction and well potentials, but it seems clear that there will be no essential change if either the interaction or the potential well has an exponential tail. This must, of course, be taken into account when choosing the limiting contours as in figs. 3 or 5. However, the reasoning used here will fail completely if Coulomb forces or other interactions varying as a power of the distance are to be taken into account.

This work, begun in Oxford, was completed in the National University of Mexico. One of the authors (G.G.-C.) would like to acknowledge support in Oxford from the National University of Mexico and the Consejo Nacional de Ciencia y Tecnología of Mexico. R.P. expresses his gratitude for hospitality in the University and the award of the Elena Aizen de Moshinsky Visiting Professorship.

References

1) H. T. Fortune and C. M. Vincent, Phys. Rev. C2 (1970) 782
2) R. Huby, Nucl. Phys. A167 (1971) 271
3) G. Gamow, Z. Phys. 51 (1928) 204
4) Y. B. Zel'dovich, JETP (Sov. Phys.) 12 (1961) 542
5) T. Berggren, Nucl. Phys. A109 (1968) 265
6) N. Hokkyo, Progr. Theor. Phys. 33 (1965) 1116
7) T. Berggren, Nucl. Phys. A169 (1971) 353
8) H. Araki, Y. Munakata, M. Kawaguchi and T. Goto, Progr. Theor. Phys. 17 (1957) 419
9) T. Goto, Progr. Theor. Phys. 21 (1959) 1
10) J. B. Scheffler, D. Phil. Thesis, Oxford (1970)
11) R. G. Newton, Scattering theory of waves and particles (McGraw-Hill, New York, 1966) ch. 12

Solid State Communications, Vol. 71, No. 4, pp.237-241, 1989.
Printed in Great Britain.

0038-1098/89$3.00+.00
Maxwell Pergamon Macmillan plc

PROPERTIES OF THE DWELL TIME AND THE TRANSMISSION AND REFLECTION TIMES FOR RESONANT TUNNELING

Gastón García-Calderón
Instituto de Física, Universidad Nacional Autónoma de México
Apartado Postal 20-364, México 01000,D.F. México

Alberto Rubio
Escuela Superior de Ciencias, Universidad Autónoma de Baja California, Apartado Postal 1880, Ensenada B.C. México

(Recieved by M. Tosi-20th September 1988)

For a one dimensional arbitrary potential profile, Breit- Wigner expressions for the phase energy-derivatives for transmission, θ', and reflection, ϕ'_{OL} and ϕ'_{LO}, -for each incident direction-, in terms of the partial decay widths Γ^O and Γ^L are derived. Consideration of these relations at resonance energy for two limiting cases -full resonant transmission (T=1) $\hbar\theta'=2\hbar/\Gamma$ and full resonant reflection (T=0) $\hbar\phi'_{OL}=4\hbar/\Gamma$, where $\Gamma=\Gamma^O+\Gamma^L$ - provide unambiguous meaning to the notion of $\hbar\theta'$ as a transmission time and of $\hbar\phi'_{OL}$ and $\hbar\phi'_{LO}$, as reflection times. We study the effect of the asymmetry of the potential on these times and obtain that reflection times may be much larger than the transmission time. A time independent derivation of the dwell time is also presented. This expression assumes the form of a weighted average, but an oscillating term also appears, confirming a result by Hauge et.al. ref.[7]. For the case of a resonance far from threshold energy, the oscillating term is small and the dwell time may be written, at each incident direction, as $\tau_{OL}=\hbar[T\theta' +R\phi'_{OL}]$ and $\tau_{LO}=\hbar[T\theta'+R\phi'_{LO}]$.

The advent of new semiconductor microstructures at nanometric scales has given rise lately to a considerable effort devoted to the understanding of electronic transport in such systems [1,2]. Transport based on resonant tunneling processes has received special attention. Particularly the times involved in these processes have been the subject matter of several recent contributions [2-9]. One should also mention a number of works mainly concerned with off-resonance tunneling times [10-16].

In a typical experimental set up the electrons have a well defined energy and therefore the solutions of the Schrödinger equation outside the interaction region are adequately represented by plane waves [17]. Hence, for arbitrary energies, the wave solutions extend through all space. If the potential profile sustains resonances, to be on or off-resonance means that the probability to find electrons within the interaction region is, respectively, very large or very small.

An appropriate quantity to measure the average time that electrons spend within the potential is the dwell time [4,5,9]. In a previous paper [9] the present authors have considered some properties of the outgoing wave propagator to derive expressions for the dwell time near resonance energy in terms of the partial decay widths, Γ^O and Γ^L, which are the relevant quantities to describe scattering near resonance in a Breit-Wigner fashion. On the other hand, Barker [5] and Hauge et.al. [7] have recently derived expressions for the dwell time, using a time dependent approach, in terms of the energy derivatives of the phases of the transmission and reflection amplitudes θ' and ϕ'. Although these two calculations differ by the presence of an oscillating term in the result of Hauge et.al. they reduce to the same form near resonance energy [7].

It is the main purpose of this work to establish a relationship between the partial decay widths [9] and the energy-derivatives of the phases evaluated at resonance energy. This leads to a connection between both ways of expressing the dwell time. We discuss the importance of this in relation to the roles of the transmission, reflection and dwell times in one dimensional resonant tunneling.

We also present a derivation for the dwell time in terms of the phase derivatives, for transmission and reflection, alternative to that of refs. [5] and [7]. This derivation is time independent and leads to the same expression obtained by Hauge et.al.[7].

Let us first consider the time independent derivation of the dwell time in terms of the energy derivatives of the phases of the transmission and reflection amplitudes. In doing so we apply an argument involving Green's theorem and the Schrödinger equations for ψ and $\partial\psi(E,x)/\partial E$ [18]. Consider the Schrödinger equation for an electron of mass m and energy E incident from the left, $x<0$,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(E,x)+[V(x)-E]\psi(E,x)=0 \qquad (1)$$

where $V(x)$ is an arbitrary potential profile in one dimension which vanishes in the region $x\leq 0$ and $x\geq L$. Beyond the range of interaction the solutions to eq.(1) may be written in the usual form, $\psi(E,x) = t(k)\exp(ikx)$, and $\psi(E,x)= \exp(ikx)+r(k)\exp(-ikx)$, respectively, for $x\geq L$ and $x\leq 0$. Here $\kappa=(2mE)^{1/2}/\hbar$, and $t(k)$ and $r(k)$ stand for the transmission and reflection amplitudes. Let us write the energy derivative of eq.(1),

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)-E]\frac{\partial\psi(E,x)}{\partial E}-\psi(E,x)=0 \qquad (2)$$

multiply eq.(2) by $\psi^*(E,x)$ and substract the complex conjugate of eq.(1) times $\partial\psi(E,x)/\partial E$. Integrating the resulting expresion along the region of interaction yields, after dividing by the incident flux $J_i=\hbar k/m$, the dwell time $\tau(E)$,

$$\tau(E)=\frac{m}{\hbar k}\int_0^L|\psi|^2dx =$$

$$=-\frac{\hbar}{2k}[\psi^*\frac{\partial^2\psi}{\partial x\partial E}-(\frac{\partial\psi}{\partial E})(\frac{\partial\psi^*}{\partial x})]_0^L \qquad (3)$$

Substitution into the previous equation of the solutions of ψ at the end points $x=0$ and $x=L$ yields,

$$\tau(E)=\hbar[T\theta'+R\phi']+\frac{m}{\hbar k}[TL+\frac{R^{1/2}}{k}\sin\phi] \qquad (4)$$

Noting that our derivatives are E-derivatives and those in ref.[7] are k-derivatives, it is straightforward to see that our expression for τ, eq.(4), is identical to eq.(5.9) of Hauge et.al.[7]. It has been shown in ref.[9] that for arbitrary potential profiles there are actually two different values for the dwell time, each corresponding to one or the other incident direction. In the case of a sharp isolated resonance of total width Γ, i.e. $E_{res}>>\Gamma$ and $\Delta E >> \Gamma$ (ΔE being the distance between E_{res} and the nearest resonance) it is well known that the phase derivatives at resonance energy are very large. This is related to the fact that the electron spends a much longer time within the interaction region $0\leq x\leq L$ that the corresponding time $t_o=\hbar L/mk$ in the absence of interaction. Since, in addtion, we assume that the resonance occurs far from threshold energy ($E=0$), the contribution of the last term on the right hand side of eq.(4) may be neglected and consequently one may write,

$$\tau_{oL}(E_{res})=\hbar\,[\,T\theta'+R\phi'_{oL}\,] \qquad (5)$$

where the subindex oL in the above expression indicates that scattering is from the left. Similarly for an electron approaching the system from the right, the dwell time reads,

$$\tau_{Lo}(E_{res})=\hbar\,[\,T\theta'+R\phi'_{Lo}\,] \qquad (6)$$

In writing eqs.(5) and (6) we have made use of the properties of flux conservation and time reversal invariance of the 2x2 M-matrix associated to scattering in one dimension, which for the transmission amplitudes imply the relationship $t_{oL}=t_{Lo}=t$ and hence the corresponding phases fulfill $\theta'_{oL}=\theta'_{Lo}=\theta'$ [19,20].

In a previous paper [9] we have derived an alternative expression for the dwell times τ_{oL} and τ_{Lo}. In this approach the resonance energy and the total width correspond, respectively to the real part, E_r, and imaginary part, Γ, of a complex pole of the propagator of the problem. Near resonance energy one may write the dwell times as [9],

$$\tau_{oL}(E)=\frac{\hbar\,\Gamma^o}{(E-E_r)^2+\Gamma^2/4} \qquad (7)$$

and

$$\tau_{Lo}(E)=\frac{\hbar\,\Gamma^L}{(E-E_r)^2+\Gamma^2/4} \qquad (8)$$

where the total width $\Gamma=\Gamma^o+\Gamma^L$ and the partial decay widths Γ^o and Γ^L are associated, respectively, with the probabilities of electronic decay through the end points $x=0$ and $x=L$ of the potential profile. (Notice that in writing Γ, we have absorbed into Γ^o and Γ^L the 1/2 factor appearing in ref.[9]).

For future use we also recall the expression for the transmission coefficient, at resonance energy, in terms of the partial widths [9],

$$T(E)=\frac{\Gamma^{o}\Gamma^{L}}{(E-E_{r})^{2}+\Gamma^{2}/4} \qquad (9)$$

In order to establish a relationship betewen the phase derivatives $\theta', \phi'_{oL}, \phi'_{Lo}$ and the partial decay widths Γ^{o} and Γ^{L}, we note that eqs.(5) and (6) relate the phase derivatives to the times τ_{oL} and τ_{Lo} and in turn eqs.(7) and (8) relate these times to the partial widths. However there are three phase derivatives and only two equations. In order to solve for the phase derivatives we need an additional independent equation. This may be obtained also from the properties of flux conservation and time reversal invariance of the M-matrix, which in addition to $t_{oL}=t_{Lo}=t$, require also that $|r_{oL}|=|r_{Lo}|$ and $r_{oL}=-[t_{oL}/t^{*}_{oL}]r^{*}_{Lo}$ [20]. Hence writing the amplitudes showing their phases explicitly leads after straightforward algebra, to the third equation needed,

$$2\theta'=\phi'_{oL}+\phi'_{Lo} \qquad (10)$$

Solving the simultaneous equations (5),(6) and (10) we obtain,

$$\theta'(E)=\frac{1}{2\hbar}[\tau_{oL}+\tau_{Lo}] \qquad (11)$$

$$\phi'_{oL}(E)=\frac{1}{2\hbar}[\tau_{oL}+\tau_{Lo}+(\tau_{oL}-\tau_{Lo})/R] \qquad (12)$$

$$\phi'_{Lo}(E)=\frac{1}{2\hbar}[\tau_{oL}+\tau_{Lo}-(\tau_{oL}-\tau_{Lo})/R] \qquad (13)$$

where R is the reflection coeficient. The above solution is valid for nonzero R. When R=0, eqs.(12) and (13) become undetermined through their second term, $(\tau_{oL}-\tau_{Lo})/R$, which gives 0/0. Clearly this corresponds to a full tranmission resonance, T=1, where the phases of the reflection amplitudes have no meaning since $r_{oL}=r_{Lo}=0$. Substituting into the above equations the values of τ_{oL}, τ_{Lo} and R=1-T, from eqs.(7), (8) and (9), we obtain the phase derivatives in terms of the partial widths near resonance energy,

$$\theta'(E)=\frac{(\Gamma^{o}+\Gamma^{L})/2}{(E-E_{r})^{2}+(\Gamma^{o}+\Gamma^{L})^{2}/4} \qquad (14)$$

$$\phi'_{oL}(E)=\theta'(E)+\frac{(\Gamma^{o}-\Gamma^{L})/2}{(E-E_{r})^{2}+(\Gamma^{o}-\Gamma^{L})^{2}/4} \qquad (15)$$

$$\phi'_{Lo}(E)=\theta'(E)-\frac{(\Gamma^{o}-\Gamma^{L})/2}{(E-E_{r})^{2}+(\Gamma^{o}-\Gamma^{L})^{2}/4} \qquad (16)$$

As follows from the discussion below eq.(13), the validity of Eqs.(15) and (16) requires a nonzero R and this implies $\Gamma^{o}\neq\Gamma^{L}$. In general for an asymmetric potential profile one may write $\Gamma^{o}=\Gamma^{L}+\Delta$. The case $\Delta\equiv(\Gamma^{o}-\Gamma^{L})\ll\Gamma^{L}$, which corresponds to a slightly asymmetric potential, is interesting. Let us denote the Breit-Wigner contribution which is proportional to $(\Gamma^{o}-\Gamma^{L})$ on the right hand side of eqs.(15) and (16) by A(E); then it is easy to convince oneself, as the energy approaches resonance energy, that A(E) attains a higher value and is more sharply peaked than the $\theta'(E)$ term. More specifically, if the energy is off resonance by an amount δ, i.e. $(E-E_{r})\sim\delta$ then we find that for $\delta\sim\Gamma^{L}$, $\theta'(E)\sim 1/\Gamma^{L}\gg A(E)\sim\Delta/(\Gamma^{L})^{2}$; for $\delta\sim(\Gamma^{L}\Delta/2)^{1/2}$, $\theta'(E)\sim A(E)\sim 1/\Gamma^{L}$; and for $\delta\sim\Delta$, $\theta'(E)\sim 1/\Gamma^{L}\ll A(E)\sim 1/(\Delta)$. Hence for very small Δ we obtain that for energies around resonance energy the values of the reflection phase derivatives, given by eqs.(15) and (16), are much larger than the transmission phase derivative given by eq.(14). In the opposite limit, $\Delta\gg\Gamma^{L}$, it is easy to see that even for $\delta\sim\Delta$, $\phi'_{oL}(E)\sim 2\theta'(E)$ and $\phi'_{Lo}(E)\sim 0$. In fact, eqs.(14), (15) and (16) attain their maximum contribution at the resonance energy $E=E_{r}$,

$$\theta'=\frac{2}{\Gamma}=\frac{2}{\Gamma^{o}+\Gamma^{L}} \qquad (17)$$

$$\phi'_{oL}=\frac{2}{\Gamma^{o}+\Gamma^{L}}+\frac{2}{\Gamma^{o}-\Gamma^{L}} \qquad (18)$$

$$\phi'_{Lo}=\frac{2}{\Gamma^{o}+\Gamma^{L}}-\frac{2}{\Gamma^{o}-\Gamma^{L}} \qquad (19)$$

Where we are using the notation $\theta'=\theta'(E_{r})$, $\phi'_{oL}=\phi'_{oL}(E_{r})$ and $\phi'_{Lo}=\phi'_{Lo}(E_{r})$. We emphasize that eqs. (18) and (19) are strictly valid for $\Gamma^{o}\neq\Gamma^{L}$. One may write also Γ^{o} and Γ^{L} in terms of the phase derivatives given above as $\Gamma^{o}=(1/\theta')-1/(\theta'-\phi'_{oL})$, and $\Gamma^{L}=(1/\theta')-1/(\theta'-\phi'_{Lo})$.

There are two interesting limiting cases which follow from our results. For a symmetric potential, T=1, we have $\Gamma^{o}=\Gamma^{L}$ and hence from eqs.(5), (6) and

(17), $\tau_{OL}=\tau_{LO}=\hbar\theta'=2\hbar/\Gamma$, which confirms a result by Collins et.al.[6]. This is the resonant tunneling situation. The other limiting case occurs when we have a closed channel, say, $\Gamma^L=0$ which means that electrons can not enter or leave the system through x=L. Therefore T=0; $\tau_{OL}=\hbar\phi'_{OL}=4\hbar/\Gamma$, which corresponds to the resonant reflection situation [21], and is reminiscent of the three dimensional case for zero angular momentum [22]; and $\tau_{LO}=0$. The above two limiting cases provide unambiguous meaning to the notion of transmission and reflection times. In general, however, for arbitrary potential profiles the dwell times, as is evident from eqs.(5) and (6), depend both on the transmission and reflection phase derivatives weighted by the corresponding scattering coefficients T and R. The previous discussion suggests to write a transmission time as $\tau^t=\hbar\theta'$ and reflection times as $\tau^r_{OL}=\hbar\phi'_{OL}$ and $\tau^r_{LO}=\hbar\phi'_{LO}$. Hence at resonance energy, for each incident direction, the dwell times are given by,

$$\tau_{OL}=T\tau^t+R\tau^r_{OL} \qquad \tau_{LO}=T\tau^t+R\tau^r_{LO} \qquad (20)$$

An interesting consequence of the above considerations is that for the slightly asymmetric potential discussed above, i.e. with $\Gamma^o=\Gamma^L+\Delta$, the one for which $\Gamma^L\gg\Delta$, eqs.(17)-(19) give, respectively, for the transmission time $\tau^t\simeq\hbar/\Gamma^L$, and for the reflection times $\tau^r_{OL}\simeq 2\hbar/\Delta$ and $\tau^r_{LO}\simeq -2\hbar/\Delta$ (the minus sign here indicates a time advance). That is, the reflection times become much larger than the transmission time. As discussed above this occurs for energies within Δ of the resonance energy E_r. In fact it follows, using eq.(9), that these times correspond to a value of the reflection coefficient $R\sim \Delta^2/\Gamma^2\equiv (\Gamma^o-\Gamma^L)^2/(\Gamma^o+\Gamma^L)^2\ll 1$. Notice however that the above situation refers to a limiting case. In the other limiting case, that corresponding to a closed channel, we have obtained that the relevant reflection time is twice the transmission time. Therefore, the design of potential profiles intermediate between the above limiting cases, will always provide reflection times larger than the transmission time and may lead in the foreseeable future to experimental distinction of these times as may be expected given the recent advances in experimental techniques for time measurements [23]. On the other hand, the dwell times, for very small Δ, remain of the same order of magnitude as the transmission time since $R\tau^r_{OL}$ and $R\tau^r_{LO}$ are both of the order $\Delta/(\Gamma^L)^2\ll 1$; while for very large Δ, the dwell times are of the same order of magnitude as the reflection time since $T\tau^t$ goes like $\Gamma^L/(\Delta)^2\ll 1$.

The main results of this work are eqs.(14)-(18) and eqs.(17)-(19) which relate, respectively, the phase energy derivatives θ', ϕ'_{OL} and ϕ'_{LO}, with the partial decay widths Γ^o and Γ^L near resonance energy -in a Breit-Wigner fashion- and at resonance energy E_r. Another result refers to eqs.(5), (6) and (20) for the dwell time as a weighted average time. Our results are valid for the case of a sharp isolated resonance far from threshold energy. We must remark that for resonances near threshold the assumption that the last term of eq.(4) is small is certainly not valid. Therefore, even at resonance energy, the identification of the transmission and reflection times, respectively, as $\hbar\theta'$ and $\hbar\phi'$ may not hold in that case. This needs further study. One should mention that other approaches [10-16] have paid little attention to the situation at resonance. However, Büttiker [13] has shown that for a resonance above a symmetrical single barrier the dwell time is given by $\hbar\theta'$. The relation between these other approaches and the present work requires also further study. Another result of this work is the time independent derivation of the dwell time given by eq.(4). This derivation shows that, despite claims to the contrary, a stationary calculation gives the same results as a wave packet approach, at least for a sharply peaked wave packet in k-space.

Acknowledgment/ The authors thank the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste and, (AR), DGICSA-SEP, México, for partial support.

Bibliography.

[1] 'The Physics and Fabication of Microstructures and Microdevices' edited by M.J. Kelly and C. Weissbuch (Springer-Verlag, Berlin, 1986).

[2] F. Capasso, K. Mohammed and A.Y. Cho, IEEE J. Quantum Electron 22, 1853 (1986).

[3] K.W.H. Stevens, J. Phys. C17, 5735 (1984).

[4] B. Ricco and M.Ya. Azbel, Phys. Rev. B29, 1970 (1984).
[5] J.R.Barker, in ref[1] p.210.
[6] S. Collins, D. Lowe and J.R. Barker J.Phys. C20, 6233 (1987).
[7] E.H. Hauge, J.P. Falck and T.A. Fjeldly, Phys. Rev. B36, 4203 (1987).
[8] T.B. Bahder, C.A. Morrison and J.D. Bruno, Appl. Phys. Lett. 51, 1089, (1987).
[9] G. García-Calderon and A. Rubio, Phys. Rev. B36, 4462 (1987).
[10] A.I. Baz, Sov. J. Nucl. Phys 5, 161 (1967).
[11] V.F. Rybachenko, Sov. J. Nucl. Phys. 5, 635 (1967).
[12] M. Büttiker and R. Landauer, Phys. Rev. Lett. 49, 1739 (1982).
[13] M. Büttiker, Phys. Rev. B27, 6178 1983).
[14] D. Sokolovski and L.M. Baskin, Phys.Rev. A36, 4604 (1987).
[15] C.K. Leavens and G.C. Aers, Solid State Commun. 63, 1101, (1987) and preprint, 1988.
[16] W. Jaworski and D.M. Wardlaw, Phys. Rev. A37, 2843, (1988).
[17] R. Tsu and L. Esaki, Appl. Phys. Phys.Lett. 24, 593 (1974).
[18] F.T. Smith, Phys. Rev. 118, 349 (1960).
[19] E. Merzbacher, Quantum Mechanics (Wiley,New York 2nd edition 1970) p.86.
[20] J.P. Falck and E.H. Hauge, Phys.Rev. B38, 3287 (1988).
[21] G.García-Calderón, Solid State Commun. 62, 441 (1987).
[22] G. García-Calderon and A. Rubio, Nucl. Phys. A458, 580 (1986).
[23] J.F. Whitaker, G.A.Mourou, T.C.L.G. Sollner and W.D Goodhue, Appl. Phys. Lett., 53,385 (1988).

Solid State Communications, Vol.62,No.7, pp.441-447, 1987.
Printed in Great Britain.

0038-1098/87 $3.00 + .00

THE EFFECT OF ASYMMETRY ON RESONANT TUNNELING IN ONE DIMENSION

Gastón García-Calderón
Instituto de Física,
Universidad Nacional Autónoma de México
Apdo. Postal 20-364, México, 01000 D.F.

(Received for publication 30 January 1987 by M. Tosi)

This work considers the effect of asymmetric one-dimensional multibarrier potentials on resonant tunneling. It is shown, by using the properties of the propagator of the system, that this effect may lead to novel resonance phenomena which affect the decay properties of the quasistationary states of the system. As a consequence it is shown that in general the full width at half maximum of the transmission peak at resonance does not provide the corresponding lifetime as occurs in the symmetric case. The above considerations are illustrated by a simple analytical solvable model.

In recent times there has been an increasing interest in studying electronic transport in double barrier heterostructures [1]. It is well known, since the pionnering work by Tsu and Esaki [2] and Chang, Esaki and Tsu [3], that resonant tunneling plays the relevant role for perpendicular electronic transport in the above systems, which proceeds essentially in one dimension. The problem corresponds to the scattering of electrons by a one dimensional potential and the quantity of interest is the transmission coefficient from which the I-V characteristics may be obtained. Provided the electronic mean free path is larger than the length of the system one may restrict onself to consider only elastic processes. This is the case for typical parameters of the problem [4].

The basic physics of one dimensional resonant tunneling for a symmetric potential is well understood [5]: It corresponds to a situation where a particle of well defined energy E is incident upon the system, formed by two consecutive barriers of equal height greater than E and a classically allowed region between them. At nearly all incident

energies the particle is almost totally reflected. However in a small discrete number of energy intervals, characterized by energies E_r and corresponding widths Γ_r, the particle is actually transmitted to the other side of the system. This is the phenomenon of resonant tunneling which manifests itself as a peak of unity height in a plot of the transmission coefficient vs energy. Full transmission is achieved at $E = E_r$ and the corresponding time scale of the event is given by $t \sim \hbar/\Gamma_r$, which reflects the quasistationary nature of the process. During this time a large electronic probability density builds up in the well due to constructive interference between the waves leaking through the first barrier and those being reflected off the second one. The case of multiple barriers and wells is similar except that the sequence of internal reflections leading to the formation of a resonance is more complex. In reality the experimental situation in multibarrier heterostructures corresponds to asymmetric potentials. An interesting point here is that in general asymmetric potentials lead to a reduction of the heights of the transmission peaks at resonance energies. The theoretical explanation of this fact is usually made in terms of the transmission coefficients through each barrier [5]. However such a procedure gives no complete insight on the underlying resonant processes. Motivated by the above situation, in this work I consider an approach to resonant tunneling aimed to show how resonance levels are affected by asymmetric potentials. In particular I discuss how the lifetime and decay properties of the levels are affected by the asymmetry of the potential. A crucial feature of the approach is that it takes into account the quasistationary nature of the levels. This is usually ignored. The levels of the system are commonly calculated as if they were bound states [1,3]. On the other hand, the usual procedure to obtain the lifetime of a resonant electron is by measuring the FWHM, i.e. the full width at half maximum of the transmission peak obtained by solving numerically the Schrödinger equation of the problem. However as shown below, in the case of asymmetric potentials the lifetime of the resonant electrons is not given correctly by the FWHM of the corresponding reduced transmission peak.

A convenient way to approach the problem is via the outgoing Green's function or propagator of the problem because then one may consider the well known relationship between resonances and the complex poles of the propagator to describe processes near resonance energy [6]. Here it is well known that for every resonance the real and imaginary parts of the complex pole correspond respectively to the resonant energy and energy width described above. Let us therefore

consider an arbitrary potential extending through a region of finite length L i.e. $V(x) = 0$ for $x \leq 0$ and $x \geq L$. The solutions of the Schrödinger equation for scattering from the left, i.e. $x<0$, of a wave of energy $E = k^2$ with units $\hbar = 2m = 1$, may be written outside the interaction range in the usual form $\psi(k,x) = \exp(ikx) + r(k)\exp(-ikx)$; $x \leq 0$ and $\psi(k,x) = t(k)\exp(ikx)$; $x \geq L$, where $r(k)$ and $t(k)$ are respectively the reflection and transmission amplitudes. Here for simplicity I do not include the mass variation in the different regions. Using Green's theorem between the equation for $\psi(k,x)$ and that one for the full propagator $G^+(x,x';k)$ of the problem, which obeys outgoing boundary conditions at the end points of the system, results in the following relationship for the wave function along the internal region [7],

$$\psi(k,x) = 2ik\, G^+(0,x;k) \; ; \; 0 \leq x \leq L \quad (1)$$

By considering the solution of the wave function at $x = L$ gives the transmission amplitude as

$$t(k) = 2ik\, G^+(0,L;k)\, \exp(-ikL) \quad (2)$$

The above expression is very interesting because it relates the transmission amplitude with the propagator evaluated at the point $x = 0$ and $x' = L$. Similarly the expression for the reflection amplitude reads,

$$r(k) = 2ik\, G^+(0,0;K) - 1 \quad (3)$$

which depends only on the propagator evaluated at $x = x' = 0$. For an electron approaching the system from the right it is easily seen that the transmission and reflection propagators are given respectively by $G^+(L,0;k)$ and $G^+(L,L;k)$. The relevant point is that near a complex pole $k_n = a_n - i\, b_n$ one may write the propagator as [6,7],

$$G^+(x,x';k) = u_n(x)u_n(x')/2k_n(k - k_n) \quad (4)$$

It is well known that the functions $u_n(x)$ provide a description of the resonant eigenstates in a similar fashion to bound states. They obey the Schrödinger equation with complex eigenvalues $k_n^2 = \varepsilon_n - i\,\Gamma_n/2$ with $\varepsilon_n = a_n^2 - b_n^2$ and $\Gamma_n = 4\, a_n\, b_n$ and fulfill outgoing boundary conditions [6]. Using Green's theorem between the equations for $u_n(x)$ and $u_n^*(x)$ and using the corresponding boundary conditions gives an interesting relation for the width b_n in terms of the value of the resonant eigenstate at the end points of the system,

$$b_n = (|u_n(0)|^2 + |u_n(L)|^2)/2\, I_n \quad (5)$$

where I_n is a quantity of the order of unity [7]. The above relationship defines the partial widths $b_n^0 = |u_n(0)|^2$ and $b_n^L = |u_n(L)|^2$. The relevant point here is that the partial widths represent the coupling of the resonant eigenstate with the end points of the system. Using (4) and (5) into (2) gives the transmission coefficient near resonance as,

$$|t(k)|^2 \simeq k^2 \, b_n^o \, b_n^L / \left(a_n^2 \left[(k - a_n)^2 + (b_n^o + b_n^L)^2/4\right]\right) \quad (6)$$

The above equation generalizes the usual expression for the transmission coefficient near resonance. The difference corresponds to the appearence in (6) of the partial widths b_n^o and b_n^L. Actually for a symmetric potential it is straightforward to see that the system looks the same independently of being approached from the left or from the right. This is because $|G^+(0,0,k)|^2 = |G^+(L,L;k)|^2$ and therefore $b_n^o = b_n^L = b_n$ which leads to the usual expression for the transmission coefficient near resonance,

$$|t(k)|^2 \simeq k^2 \, b_n^2 / (a_n^2 \left[(k-a_n)^2 + b_n^2\right]) \quad (7)$$

Clearly for the asymmetric case one may have $b_n^o \neq b_n^L$ and as a consequence it is easy to convince oneself, by inspection of (6), that the value of the transmission peak will depend on the ratio between b_n^o and b_n^L. The underlying resonant process may be obtained by substituting (4) and (2) into (1) which allows one to write the probability density for the electron inside the system, near resonance, as

$$|\psi(k,x)|^2 \simeq k^2 \, b_n^o \, |u_n(x)|^2 / \left(a_n^2 \left[(k - a_n)^2 + (b_n^o + b_n^L)^2/4\right]\right) \quad (8)$$

It is easy to convince onself that the ratio between the partial widths will determine whether there is a small or a large probability for the electon inside the system. The case $b_n^o >> b_n^L$ is particularly interesting because from (6) it corresponds to very small transmission, since at resonance, $|t(a_n)|^2 \simeq b_n^L/b_n^o << 1$. However from (8) one finds a large probability for the electron inside the system. This means that the incident electron forms a long lived state within the system that decays through the incident direction. This process may be called resonant reflection. In addition one may have a number of intermediate situations [7].

In order to illustrate the above points I consider the analytical treatment of a simple double barrier system. This is the double delta shell potential $V(x) = A_o \, \delta(x) + A_L \, \delta(x-L)$. Actually it is well known that the in the above model each delta may be seen as the result of the parameters of a square barrier of height V going to infinity and width d tending to zero such that the product Vd remains constant corresponding precisely to the intensity of the delta function. For an electron approaching the system from the left, the expressions for the transmission and reflection propagators follow from the corresponding integral equation in terms of the free particle Green's function $G_o^+(x,x';k) = \exp(ik|x-x'|)/2ik$. They are easily seen to correspond to

$$G^+(0,L;k) = 2ik \exp(\mp ikL)/ J(k) \quad (9)$$

and

$$G^{+}(0,0;k) = (2ik + A_L\,(\exp(2ikL) - 1))/\,J(k) \qquad (10)$$

where $J(k) = (2ik)^2 - (A_0 + A_L)2ik - A_0A_L\,(\exp(2ikL) - 1)$. The poles of $G^{+}(x,x';k)$ correspond to the zeroes of $J(k)$). Since sharp resonances require sufficiently high barriers, or in this case, large intensities, it is easy to see that under the condition where both A_0 and A_L are much larger than unity the following approximate analytic solutions are obtained for the poles $k_n = a_n - i\,b_n$.

$$k_n = n\pi\,[1-(A_0 + A_L)/LA_0\,A_L\,]/\,L - i\,[n\pi(A_0 + A_L)/\,A_0\,A_L\,]^2/L^3 \qquad (11)$$

where $n=1,2,3,\ldots$. The above expressions are a good approximation for the first quasilevels. Since the Schrödinger equation is analytic in the parameters A_0 and A_L, one may consider the limit in which both A_0 and A_L tend to an infinite value. That leads to the elementary text book result for the box of infinite walls with eigenvalues $k_n=n\pi/L$. Since $\epsilon_n=k_n^2$ one may obtain from (11) the energy shift $\Delta\epsilon_n$ and the width Γ_n for every eigenstate. For sufficiently large intensities one always obtains $\Delta\epsilon_n>>\Gamma_n$ and also $\epsilon_n>>\Gamma_n$. Using (5) and (11) allows one to write the partial decay widths b_n^0 and b_n^L, respectively as

$$b_n^0 = 2\,(n\pi)^2(\,1\,/\,A_0^2 + 1\,/\,A_0\,A_L)/L^3\,;$$

$$b_n^L = 2(n\pi)^2(\,1\,/\,A_L^2 + 1/\,A_0\,A_L)/L^3 \qquad (12)$$

As expected the partial widths, which represent the coupling of the corresponding resonant eigenstate to the end points of the system, depend on the parameters involving both barriers. As pointed out above the relevant quantity is the ratio b_n^L/b_n^0, which using (12) becomes, to leading order in the intensities,

$$b_n^L/b_n^0 = A_0/A_L \qquad (13)$$

In the symmetric case $A_0 = A_L = A$ one sees from (13) that $b_n^0 = b_n^L$ and hence it follows from (7), as expected, that $|t|^2 = 1$ at the resonance value $k = a_n$. It is well known that the above situation is independent of the well width L and depends only on the equality of the barrier intensities [5]. The interesting situations occur for the asymmetric case $A_0 \neq A_L$. Actually if $A_L/A_0>>1$ one sees from (13), that $b_n^0>>b_n^L$ and this leads, using (6), to the reduced value for the transmission peak at resonance $|t(a_n)|^2\sim A_0/A_L<<1$. The same conclusion is obtained from the exact expressions for the transmission and reflection propagators given by (8) and (9): One sees that the transmission Green's function becomes proportional to $1/A_L$, which reduces the value for the transmission, whereas the reflection Green's function becomes essentially independent of A_L. The above example illustrates that an asymmetric potential may sustain

resonance quasilevels which do not lead to a significant resonant tunneling effect. As pointed out above this corresponds to the occurence of reflection resonances.

Alternatively if $A_o/A_L>>1$, a similar analysis shows that both the transmission and reflection propagators become proportional to $1/A_o$. This corresponds to the usual reflection situation in which the electron is reflected at the boundary of the system. For a particle approaching the system from the right the transmission propagator remains the same, as may be seen from (9). However the reflection propagator becomes different. One has to interchange in (10) A_L with A_o and as a consequence the above discussion becomes reversed.

Final remarks: The main result of this work is that for an arbitrary potential the transmission peak at resonance depends on the ratio of the corresponding partial decay widths, namely,

$$|t(a_n)|^2 = b_n^o\, b_n^L/b_n^2 \qquad (14)$$

since from (5), $b_n=(b_n^o + b_n^L)/2$, it follows that a knowledge of b_n [8] and the value of the transmission peak at resonance suffices to determine both b_n^o and b_n^L in a practical way. For symmetric potentials $b_n^o = b_n^L$ and one obtains the familiar resonant tunneling situation. However for asymmetric potentials the partial decay widths are in general different and therefore responsible for the observed reduction of the transmission peak [1]. An important consequence of the above considerations is that the full width at half maximium of transmission peaks whose value is less than unity, does not provide as is usually assumed [1], the lifetime of the corresponding resonance levels. It is also found that the underlying resonant processes may lead to novel phenomena as resonant reflection. Since perpendicular electronic transport in heterostructures proceeds mainly through resonant levels, the existence of resonant reflection may be seen as an unwelcome feature of the asymmetry of the potential. Clearly one may expect these processes to gain in importance for multibarrier heterostructures.

"Acknowledgment"/ It is a pleasure to thank The International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste, where this work was initiated.

References

[1] T.C.L.G. Sollner, W.D. Goddhue, P.E. Tannenwald, C.D. Parker and D.D. Peck, Appl. Phys. Lett. 43, 588 (1983); T.J. Shewchuk, P.C. Chapin, P.D. Coleman, W. Kopp, R. Fisher and H. Morkoc, Appl. Phys. Lett. 46, 508 (1985); M. Tsuchiya and H. Sakaki, Jpn. J. Appl. Phys. 25, L185, (1986).

[2] R. Tsu and L. Esaki, Appl. Phys. Lett. 22, 562 (1973).

[3] L.L. Chang, L. Esaki and R. Tsu, Appl. Phys. Lett. 24, 593 (1974).

[4] L. Esaki, L.L. Chang, W.E. Howard and V.L. Rideout, in Proceedings of the Eleventh International Conference on the Physics of Semiconductors, Warsaw, Poland, 1972, edited by The Poland Academy of Sciences (PWN-Polish Scientific Publishers, Warsaw, Poland, 1972), p. 431.

[5] E.O. Kane in "Tunneling Phenomena in Solids", ed. E. Burstein and S. Lundqvist (Plenum press, New York 1969) pg. 9-11; B. Ricco and M. Ya. Azbel, Phys. Rev. B29, 1970 (1984); M.J. Kelly in "The Physics and Fabrication of Microstructures and Microdevices", ed. M.J. Kelly and C. Weisbuch (Springer-Verlag, N.Y., 1986 p. 174).

[6] G. García-Calderón and R.E. Peierls, Nucl. Phys. A265, 443, (1976).

[7] G. García-Calderón, ICTP Preprint IC/86/195.

[8] M. Ferrari, V. Grecchi and F. Zironi, J. Phys. C 18, 5825 (1985).