Tunneling and Tunnel Diodes

The tunnel diode is associated with the quantum tunneling phenomenon. The tunneling time through the device is very short → millimeter range applications up to 1 Tm².

Except of tunneling

If E is supposed fixed, (p close), and since we know that the particle is in the box of size Δx → ΔEΔp = 0

contradicting Heisenberg's principle ΔEΔp > \frac{h}{2} \rightarrow Tunneling through the wall takes place Δp ≠ 0

For tunneling to occur, the de Broglie wavelength of the object should be comparable with the width of the potential barrier.

The quantitative analysis of tunneling starts with Schrödinger's equation

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

\[\psi(0) = \psi(0) \neq 0\]

\[\frac{dJ}{dz} + \frac{2Q}{z}J = 0\]
e) Simple rectangular barrier

\[ T \left( \frac{E}{E_{inc}} \right) \]

Incident + reflected

\[ T \left( \frac{E}{E_{inc}} \right) \]

Transmitted

\[ T \left( \frac{E}{E_{inc}} \right) \]

\[ R \left( \frac{E}{E_{inc}} \right) \]

\[ \left| T \right|^2 = \frac{\text{Transmit}}{\text{Incident}} \]

\[ \left| R \right|^2 = \frac{\text{Reflect}}{\text{Incident}} \]

\[ 4(\xi) = \xi e^{\frac{j k \xi}{E_{inc}}} + R e^{\frac{j k (\xi - L)}{E_{inc}}} \quad \xi < 0 \]

\[ 4(\xi) = T e^{\frac{j k (\xi - L)}{E_{inc}}} \quad \xi > 0 \]

\[ k = \sqrt{2m^* \frac{E_{inc}}{\hbar^2}} \]

Inside the potential barrier

\[ -\frac{\hbar^2}{2m^*} \frac{d^2}{d\xi^2} 4 + q V_0 4 = E 4 \]

\[ \frac{d^2 4}{d\xi^2} = \frac{2m^* (q V_0 - E)}{\hbar^2} 4 \Rightarrow \frac{d^2 4}{d\xi^2} + \beta^2 4 = 0 \]

\[ \beta = \sqrt{\frac{2m^*}{\hbar^2} (q V_0 - E)} \]

For \( E < q V_0 \),

\[ 4(\xi) = F e^{\frac{\beta \xi}{E_{inc}}} + G e^{-\frac{\beta \xi}{E_{inc}}} \]

The continuity of \( 4 \) and \( \frac{d4}{d\xi} \) at \( \xi = 0 \) \& \( \xi = L \) provides \( 4 \) relations between the coefficients \( F, R, T, G \). After a lot of algebra, we get the transmission coefficient

\[ \left| T \right|^2 = \frac{4E(q V_0 - E)}{4E(q V_0 - E) + (q V_0)^2 \pi \hbar^2 \left[ 2m(q V_0 - E) \right]^2} \left[ \frac{L}{L} \right] \]

\( \left| T \right|^2 \) decreases monotonically as \( E \) decreases. When \( \beta L \gg 1 \)

\( \left| T \right|^2 \) becomes quite small and varies as \( \exp \left( -\frac{2\beta L}{E} \right) \)

have a finite transmission coefficient, we require a small tunneling distance \( L \), a low potential barrier \( q V_0 \), and a small effective mass.
Boundary value + Self-consistent I-V curves.

\[ E_c(z) \]

\[ z = 0 \quad z = L \]

\[ \psi(x) = \text{solution of Schrödinger equation} \]
\[ = \phi(x) e^{i \frac{1}{2} \frac{z}{\hbar}} \quad \hat{z} = (x, \hat{y}) \]

\[ \frac{d^2 \phi(x)}{dz^2} + \frac{2m^*}{\hbar^2} \left( E - E_t - E_c(z) \right) \phi(x) = 0 \]

\[ E_t = \frac{1}{2} \frac{\hbar^2}{2m^*} = \text{Transverse kinetic energy} \]

Use Transfer matrix approach and calculate everywhere \( \frac{d\phi}{dz} \) assuming these 2 quantities.

The BC are for the 2 fluxes of electrons impinging from opposite contacts.

1. BC for \( z = 0 \):
   - \( e^{ikz} \)
   - \( e^{-ikz} \)
   - \( + R e^{-ikz} \)

2. BC for \( z = L \):
   - \( T e^{ikL} \)
   - \( e^{-ikL} \)
   - \( + R e^{ikL} \)

Both \( \psi_{l-n}(z) \) & \( \psi_{n-l}(z) \) are calculated using the Transfer matrix approach.
Problem. Find Transfer Matrix for a region where both \( E_c(z) \) and effective mass are constants.

\[
\frac{d}{dz} \left( \frac{1}{f(z)} \frac{df}{dz} \right) + \frac{2m_e}{\hbar^2} \left[ E - \frac{E_T}{\hbar c} - E_c \right] \phi(z) = 0 \tag{D.85}
\]

\[ f(z) = M(z) \quad E_c = \frac{\hbar^2 k_t^2}{2m_e c^2} \quad E = E_P + E_T \quad E_P = \frac{\hbar^2 k_t^2}{2m_e c}
\]

The effective mass is contact.

We search solutions of this equation such that

\[ \phi(0) = A_1 \quad \phi'(0) = A_2 \]

\[ \phi''(0) = A_1 \quad \phi'(0) = A_2 \]

where the prime denotes first derivative with respect to space. The solutions \( \phi_1(z), \phi_2(z) \) are linearly independent (their Wronskian is unity). A general solution of the equation (D.85) above can be written as

\[ \phi(z) = A_1 \phi_1(z) + A_2 \phi_2(z) \]

The transfer matrix is defined as follows

\[
\begin{bmatrix}
\phi'(L) \\
\phi(L)
\end{bmatrix} = W \begin{bmatrix}
\phi'(0) \\
\phi(0)
\end{bmatrix}
\]

\[ W = \begin{bmatrix}
\frac{\phi_1(L)}{f} & \frac{\phi_2(L)}{f} \\
-f \phi_1(L) & f \phi_2(L)
\end{bmatrix}
\]

\[ \text{det} W = 1 \quad \text{(remember } W \text{ is independent of } z) \]
The explicit forms for $m_{1,2}(z)$ are the following:

**Case 1**  \[ E > \frac{E_{r}}{\delta} + E_{c} \]

\[ m_{1}(z) = \frac{\sinh \beta z}{\beta} \]

\[ m_{2}(z) = \cos \beta z \]

where \( \beta^{2} = \frac{2m}{\hbar^{2}} \left[ E - \frac{E_{r}}{\delta} - E_{c} \right] \)

**Case 2**  \[ E < \frac{E_{r}}{\delta} + E_{c} \]

\[ m_{1}(z) = \frac{1}{\delta} \sinh (kz) \]

\[ m_{2}(z) = \cosh (kz) \]

where \( k^{2} = \frac{2m}{\hbar^{2}} \left[ \frac{E_{r}}{\delta} + E_{c} - E \right] \)
\[-\frac{\hbar^2}{2m^*(z)} \frac{\partial^2 \psi}{\partial x^2} - \frac{\hbar^2}{2m^*(z)} \frac{\partial^2 \psi}{\partial y^2} - \frac{\hbar^2}{2m^*(z)} \frac{\partial^2 \psi}{\partial z^2} \]

\[+ E_c(z) \psi = E' \psi \]

$m^*(z)$ is spatially varying effective mass

$\psi(x, y, z) = \phi(z) e^{ik \cdot r}$

\[\frac{d}{dz} \left[ \frac{1}{f(z)} \frac{d\phi}{dz} \right] + \frac{2m_c^*}{\hbar^2} \int E_T + E_E [1 - f^{-1}(z)] - E_c(z) \phi(z) = 0 \]

\[j(z) = m^*(z)/m_c^* \]

\[E_T = \frac{\hbar^2 k_T^2}{2m_c^*} \]

\[E_P = \frac{\hbar^2 k_P^2}{2m_c^*} \]

\[\text{On the contacts} \]

\[\text{Density of States} \]

\[L \times \frac{2\pi n y}{L} \]

\[\text{Bloch Theorem} \]

\[\psi = e^{i k x \cdot r} \phi(x) \quad \phi(x + L) = \phi(x) \quad (\text{same for } k_y, k_z = \frac{n_y, n_z}{L}) \]

\[n_x = 0, \pm 1, \pm 2 \]

\[1 \text{ state in } \frac{(2\pi n_y)^3}{L^3} \]

\[\text{Density of States} \quad \frac{L^3}{(2\pi)^3} \int d^3 k \]

\[\text{for spin is taken into account} \]

\[\text{Density of States} \quad \frac{L^3}{(2\pi)^3} \int d^3 k \]
The total charge density at any point $z$ inside the device is then obtained by adding the total charge density associated with two oppositely flowing currents. For the particles impinging from the left, we have a total charge density given by

$$n^L(z) = \frac{1}{4\pi^2} \int \frac{d^3k}{(2\pi)^3} \left| \psi^L_k(z) \right|^2 \nu(E_k)$$

where $\nu(E_k) = \left[ 1 + e^{(E_k - E_F)/k_BT} \right]^{-1}$

is the Fermi-Dirac factor and $E_k = E_c(0) + \frac{\hbar^2 k^2}{2m^*}$

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

with $E_c(0)$ being the bottom of the conduction band in the left contact, which is later taken as a reference point.

Note $\psi^L_k$ depends on the transverse energy $E_T$, complicating the integration above $\int d^3k$. In practice, $E_T$ is replaced by its thermal average $k_BT$ in solving the Schrödinger equation. The wavefunction can then be recovered from the integration over transverse momentum,

$$n^L(z) = \int_{0}^{+\infty} \frac{dk_z}{2\pi} \left| \psi^L_{k_z}(z) \right|^2 \int_{0}^{+\infty} \frac{dk_T}{k_BT} \left[ \exp \left( \frac{E_c(0) - E_F}{k_BT} + \frac{\hbar^2 k^2}{2m^*} \right) \right]^{-1}$$

The $\int$ over $k_T$ can then be performed. One obtains

$$n^L(z) = \int_{0}^{+\infty} \frac{dk_z}{2\pi} \left| \psi^L_{k_z}(z) \right|^2 \sigma^L_{k_z}$$

where

$$\sigma^L_{k_z} = \frac{m^* k_BT}{\pi \hbar^2} \ln \left[ 1 + \exp \left( \frac{E_c(0) - E_F}{k_BT} + \frac{\hbar^2 k^2}{2m^*} \right) \right]$$

Following a similar derivation, the charge density associated with the flow of electrons impinging from the right contact is given by an expression similar to (508) above with the simple substitutions

$$\left| \psi^L_{k_z}(z) \right|^2 \rightarrow \left| \psi^R_{k_z}(z) \right|^2$$

$$\sigma^L_{k_z} \rightarrow \sigma^R_{k_z} = \sigma^L - \sigma^R$$

with the replacement of $E_c(0)$ by $E_c(L)$. 

The total charge density is then given by

$$n(z) = n^L(z) + n^R(z)$$
18. On page 34 of the notes, it was shown that

\[ \chi^{L-R}(z) = \int_{0}^{\infty} \frac{dk_{z}}{2\pi} \int_{0}^{\infty} \frac{dk_{t}}{2\pi} \frac{\exp\left[\left(\frac{E_{c}(0) - E_{f} + \frac{\hbar^{2}}{2m^{*}} (k_{z}^{2} + k_{t}^{2})}{k_{B}T}\right)} + 1\right]}{k_{B}T}. \]

Perform the integration over \( k_{t} \) and show that

\[ \chi^{L-R}(z) = \int_{0}^{\infty} \frac{dk_{z}}{2\pi} \left| \Phi^{L-R}(z) \right|^{2} \sigma^{L-R}(k_{z}) \]

where

\[ \sigma^{L-R}(k_{z}) = \frac{m^{*}}{\pi \hbar} k_{B}T \ln\left[1 + \exp\left(\frac{E_{f} - E_{c}(0) - \frac{\hbar^{2} k_{z}^{2}}{2m^{*}}}{k_{B}T}\right) + 1\right] \]

\[ \sigma^{L-R}(k_{z}) = \int_{0}^{\infty} \frac{dk_{t}}{\pi} \left[ \exp\left(\frac{E'}{k_{B}T} + \frac{\hbar^{2}}{2m^{*}} k_{t}^{2}/k_{B}T\right) + 1\right]^{-1} \]

\[ = \int_{0}^{\infty} \frac{dk_{t}}{2\pi} \left[ \exp\left(\frac{E' + \frac{\hbar^{2}}{2m^{*}} k_{t}^{2}}{k_{B}T} + 1\right)\right]^{-1} \]

\[ (E' = E_{c}(0) - E_{f} + \frac{\hbar^{2} k_{z}^{2}}{2m^{*}}) \]

\[ = \frac{2m^{*} k_{B}T}{\hbar} \int_{0}^{\infty} \frac{dx}{2\pi \left(1 + e^{x}\right)} \quad (x = \frac{\frac{\hbar^{2}}{2m^{*}} k_{z}^{2} + E'}{k_{B}T}) \]

\[ = \frac{m^{*} k_{B}T}{\hbar \pi} \int_{E'}^{\infty} \frac{dx}{1 + e^{x}} \]

\[ = \frac{m^{*} k_{B}T}{\hbar \pi} \left[ \ln\left(1 + e^{E'}/k_{B}T\right) \right] \]

\[ = \left(\frac{m^{*} k_{B}T}{\hbar \pi}\right) \ln\left(1 + e^{E'}/k_{B}T\right) \]

\[ = \left(\frac{m^{*} k_{B}T}{\hbar \pi}\right) \ln\left[1 + \exp\left(\frac{E_{f} - E_{c}(0) - \frac{\hbar^{2} k_{z}^{2}}{2m^{*}}}{k_{B}T}\right)\right] \]

\~35~
The total electron density is then calculated by adding the two previous contributions
\[ n(z) = n^1(z) + n^2(z). \]

### Electrionic potential

The Poisson equation to be solved written in its more general form is
\[ \frac{d^2(E(z))}{dz^2} + q \left[ N_0^+(z) - N_n^-(z) - n(z) + p(z) \right] \]

In solving that equation, we have to impose the continuity of \( \phi(z) \) and \( \varepsilon(z) \frac{d\phi(z)}{dz} \)

### Calculation of Current density

#### for components

\[ J = \frac{1}{2 e m v} \left[ 4 \phi \frac{d\phi}{dz} - 4 \phi \frac{d\phi}{dz} \right] \]

#### where
\[ T^2 = \frac{k_B T}{k_B (2\pi)} \]

Similarly we calculate \( J \) associated to the stream of electrons going from right to left. The total current density through the device is then given by
\[ J = J^2 \frac{1}{2 e m v} \]

The set of the equations described above must be solved self-consistently. Typically 10-15 iterations are necessary. The difficulty of this technique when applied to RTD's is in the precise calculation and determination of the resonant peaks in the transmission coefficients (see examples).
Resonant Tunneling Structures

Qualitative Explanation of NDR in I-V curve of RTD's!

Figure 1.3 Negative differential resistance as a consequence of conservation of transverse momentum.
Numerical Implementation

START

Read in device

Compute: $n^{l-r}, j^{l-r}$

Compute: $n^{r-l}, j^{r-l}$

Compute new potential $\Phi$

$n = n^{l-r} + n^{r-l}$

$J = J^{l-r} - J^{r-l}$

Iterate?  

Y  

N  

END

SELF CONSISTENT CALCULATIONS
CALCULATION of THE CHARGE DENSITY

For the particles impinging from the left, we have a total charge density given by

\[ n^{1-r}(z) = \frac{1}{4\pi^3} \int d^3k \ | \psi_{k}^{1-r}(z) |^2 f(E_k) \]

\[ E_k = \frac{\hbar^2 k^2}{2m^*_c} + E_C(0) \]

\[ n^{1-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} | \psi_{k_z,k_BT}(z) |^2 \int_0^{+\infty} \frac{dk_x}{2\pi} \exp[(E_C(0) - E_f + \frac{\hbar^2}{2m^*_c}(k_x^2+k_y^2))/k_BT] + 1]^{-1} \]

\[ n^{1-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} | \psi_{k_z,k_BT}(z) |^2 o^{1-r}(k_z) \]

\[ o^{1-r}(k_z) = \frac{m^*_c k_BT}{\pi \hbar^2} \ln[1 + \exp[(E_f - E_C(0) - \hbar^2 k_z^2/2m^*_c)/k_BT]] \]
CALCULATION of CURRENT DENSITY

For particles from the left contact we have a current density given by

\[ J^{l-r} = -\frac{q \hbar}{m_e \pi} \int_0^{+\infty} \frac{dk_z}{2\pi} k_z T^{l-r}(k_z) \int_0^{+\infty} dk_z k_z f(E_k) \]

\[ T^{l-r}(k_z) = \frac{k_z(L)}{k_z(0)} \left| \psi_{k_z(0),k_{\beta}(L)}^{l-r} \right|^2 \]

\[ J^{l-r} = -\frac{q \hbar}{m_e} \int_0^{+\infty} \frac{dk_z}{2\pi} k_z T^{l-r}(k_z) \sigma^{l-r}(k_z) \]

and by analogy, for electrons incident from the right contact,

\[ J^{r-l} = -\frac{q \hbar}{m_e} \int_0^{+\infty} \frac{dk_z}{2\pi} k_z T^{r-l}(k_z) \sigma^{r-l}(k_z) \]

Total current density \( J \), is then the difference of the two oppositely flowing currents.

\[ J = J^{l-r} - J^{r-l} \]
CALCULATION of the
ELECTROSTATIC POTENTIAL

The Poisson equation, written in its more general form, is

\[
\frac{d}{dz} (\epsilon(z) \frac{d}{dz} \Phi(z)) = +q \left[ N_D^+(z) - N_A^+(z) - n(z) + p(z) \right]
\]

In solving this equation, we have to impose the continuity of

\[
\Phi(z) \text{ and } \epsilon(z) \frac{d}{dz} \Phi(z)
\]

Poisson and Schrödinger equations are then solved iteratively until a self-consistent solution is obtained.
A TYPICAL DEVICE
( RAY and RUDEN )

Example Calculations:
50 ÅSpacer Layers

\[ \text{Conduction Band Energy (eV)} \]

- self-consistent
- flatband

\[ \text{Electron Density (cm}^{-3}) \]

- self-consistent
- flatband

\[ \text{Position (Angstroms)} \]
FIG. 1. (a) Structure fabricated by Ray et al. (Ref. 4). Contact regions are GaAs doped $2 \times 10^{18}$ cm$^{-3}$ (Te); spacer regions are undoped GaAs; barriers are undoped Al$_{0.4}$Ga$_{0.6}$As; and the well is undoped GaAs. (b) Equilibrium conduction-band profiles for self-consistent and flatband calculations.

FIG. 2. Current-voltage characteristics (both self-consistent and flatband results) for the structure of Fig. 1, at 300 K. Note that the inclusion of self-consistency has shifted the position of NDR to a higher bias, and broadened the characteristic. In addition, the peak current is reduced for the self-consistent calculation.

FIG. 3. Conduction-band profile for biases of current maxima, for (a) flatband analysis (point $P$ of Fig. 2) and (b) self-consistent analysis (point $Q$ of Fig. 2). The level of the quasi-bound state is well above the conduction band edge in the contact, for the self-consistent case.
Example Calculations:
500 Å Spacer Layers

Predict: $I_{\text{max layer}}$; $V_{\text{NDR}}$ higher!
Figure 2.16  SC conduction band profile for the structure with 500 Å spacer layers, at 300° K. The structure is under a bias corresponding to the SC peak current. Any further application of bias causes the quasi-bound state to be "shadowed" by the SC electrostatic potential.
Figure 2.15  Current-voltage characteristics (both SC and NSC calculations) for the structure with 500 Å spacer layers, at 300 °K.
Figure 2.17  Comparison of the SC I-V characteristic and that obtained experimentally by Ray, for the structure with 500 Å spacer layers, at 300° K. Any interpretation of this data should be made with care, since a variety of experimental unknowns can significantly affect results.