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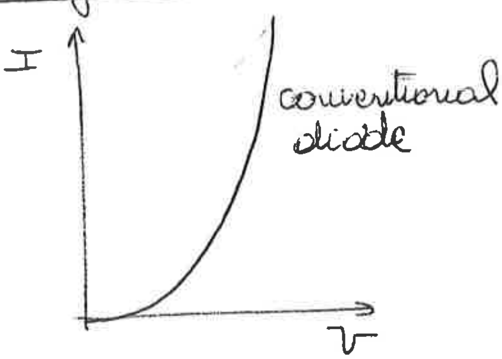
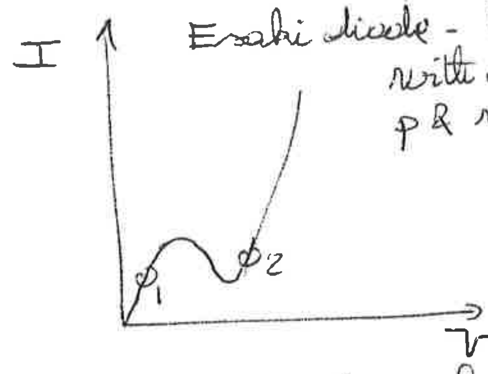
To:

Date:

From:

Tunneling and Tunnel Diodes

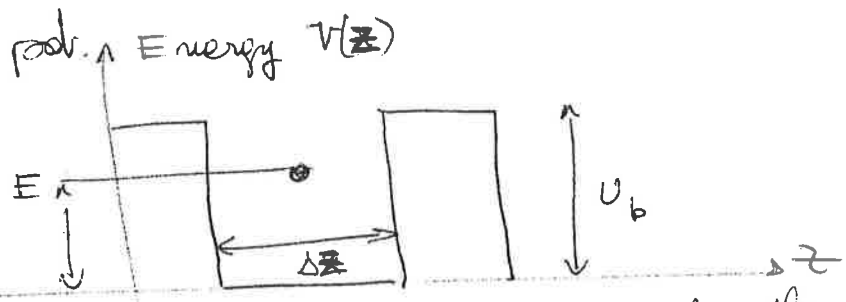




Esaki diode - tunnel diode with degenerate p & n sides.

The tunnel diode is associated with the quantum tunneling phenomena. The tunneling time through the device is very short $\longrightarrow$ millimeter range applications up to 1 THz.

Concept of tunneling



If E is supposed fixed, (p also), and since we know that the particle is in the box of size $\Delta z \Longrightarrow \Delta z \Delta p \doteq 0$ contradicting Heisenberg's principle $\Delta z \Delta p > \frac{\hbar}{2} \Rightarrow$ Tunneling through the wall takes place $\Delta p \neq 0$

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 Schroedinger's equation

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dz^2} + V(z)\psi = E\psi$$

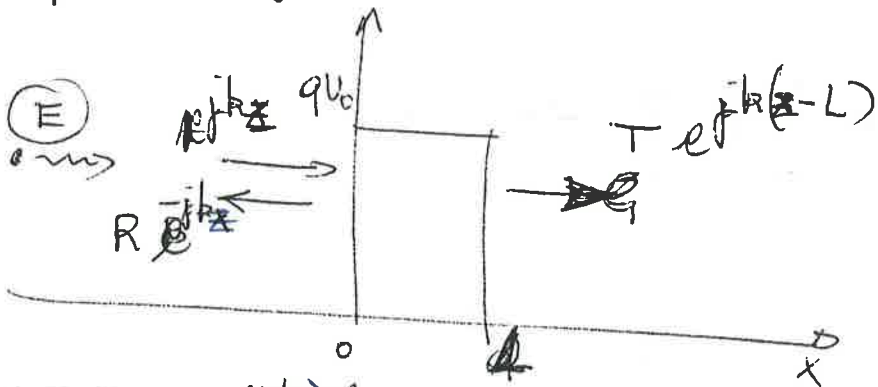
$\rho = \psi^*\psi$

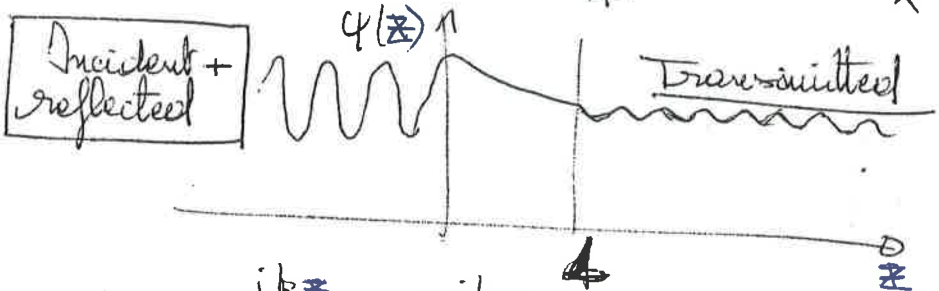
$J_z = \frac{\hbar}{2m^* i}\left(\psi^*\frac{d\psi}{dz} - \psi\frac{d\psi^*}{dz}\right)$

$\vec{J} =$

$$\boxed{\frac{d}{dz}J_z + \frac{\partial \rho}{\partial t} = 0}$$

a) Simple rectangular barrier





$$|T|^2 = \frac{J_{trans}}{J_{inc}}$$

$$|R|^2 = \frac{J_{refl}}{J_{inc}}$$

$$\psi(z) = A e^{jkz} + R e^{-jkz} \qquad z \leq 0$$
$$\psi(z) = T e^{jk(z-L)} \qquad z \geq L$$

$$k = \sqrt{\frac{2m^* E}{\hbar^2}}$$

Inside the potential barrier

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi + qV_0\psi = E\psi$$

$$\frac{d^2\psi}{dz^2} = +\frac{2m^*}{\hbar^2}(qV_0 - E)\psi \implies \frac{d^2\psi}{dz^2} - \beta^2\psi = 0$$

where

for $E < qV_0$, $\psi(z) = F e^{\beta z} + G e^{-\beta z}$

$$\beta = \sqrt{\frac{2m^*}{\hbar^2}(qV_0 - E)}$$

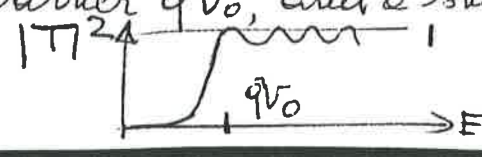
The continuity of ψ and $\frac{d\psi}{dz}$ at $z=0$ & $z=L$ provides 4 relations between the coefficients A, R, T, F & G. After a lot of algebra, we get the transmission coefficient

$$|T|^2 = \frac{4E(qV_0 - E)}{4E(qV_0 - E) + (qV_0)^2 \sinh^2\left[\frac{1}{\hbar}\sqrt{2m(qV_0 - E)}\, L\right]}$$

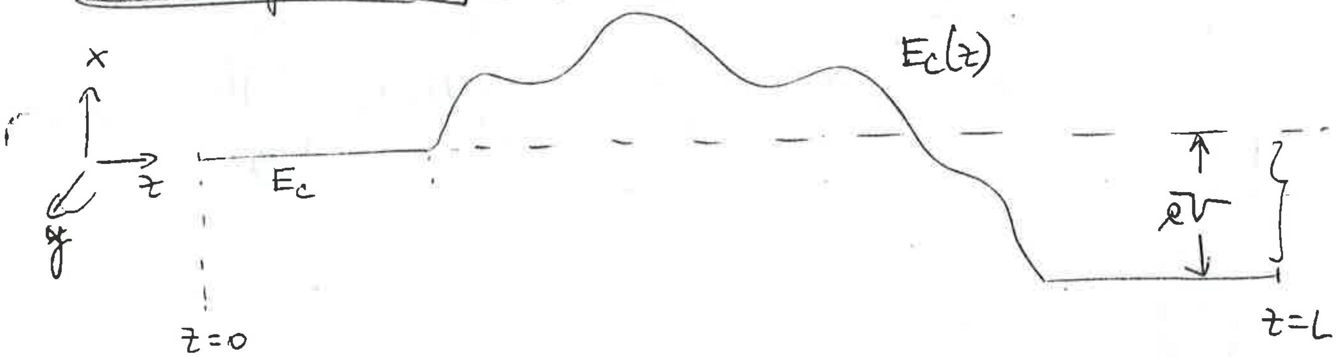
$|T|^2$ decreases monotonically as E decreases. when $\beta L >> 1$

$|T|^2$ becomes quite small & varies as $\sim \exp(-2\beta L)$

have a finite transmission coefficient, we require a small tunneling distance L, a low potential barrier qV_0, and a small effective mass.



Boundary value + Self-consistent I–V curves.



$\psi(\vec{r})$ = solution of Schroedinger equation (3D)

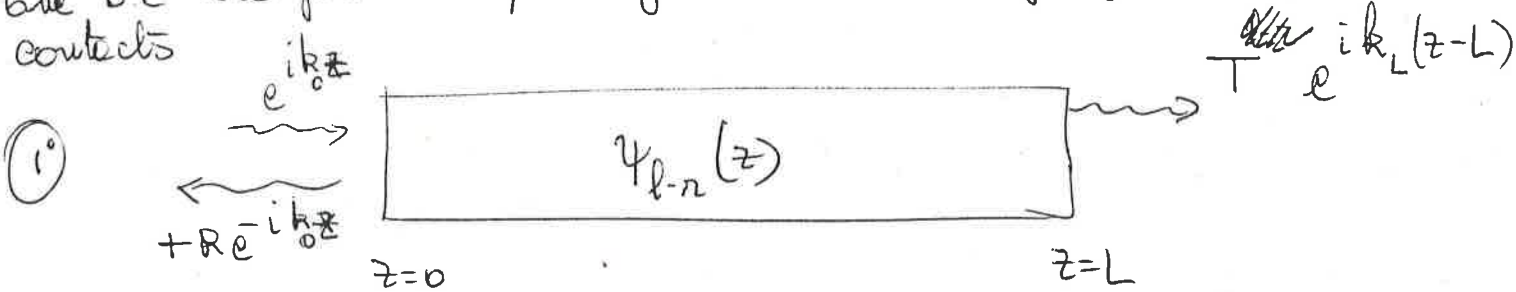
$$= \phi(z)\, e^{i\vec{k}_t \cdot \vec{r}} \qquad \vec{r} = (x, y)$$

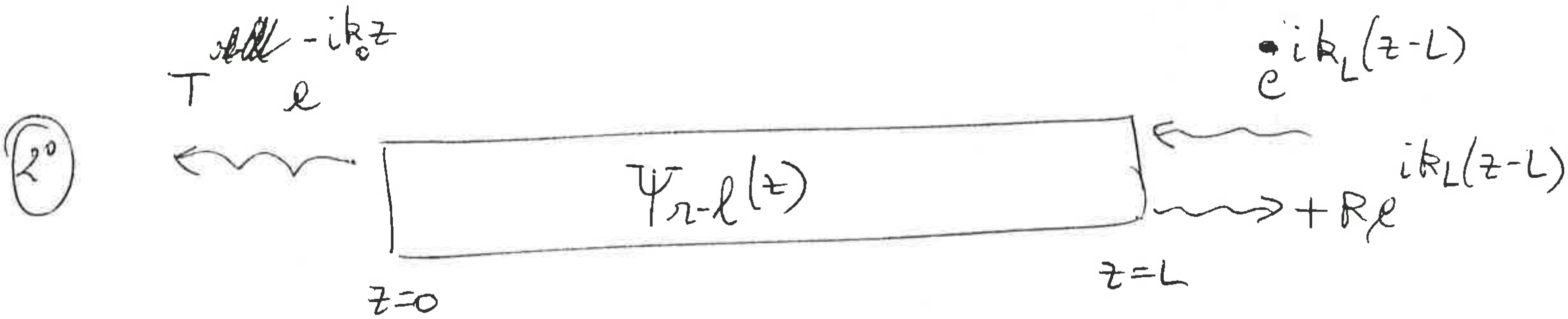
$$\frac{d^2}{dz^2}\phi(z) + \frac{2m^*}{\hbar^2}\left(E - E_t - E_c(z)\right)\phi(z) = 0$$

$$E_t = \frac{\hbar^2 k_t^2}{2m^*} = \text{Transverse kinetic energy}$$

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

The B C are for the 2 fluxes of electrons impinging from opposite contacts





Both $\psi_{l-r}(z)$ & $\psi_{r-l}(z)$ are calculated using the transfer matrix approach.

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$$\left[-\frac{\hbar^2}{2m_{\parallel}^*}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m^*(z)}\right)\frac{d}{dz}\right]\psi(\vec{r}) + E_c(z)\phi(z) = E\psi(\vec{r})$$

$$\psi(\vec{r}) = e^{i\vec{k}_t\cdot\vec{r}}\phi(z)$$

Problem. Find Transfer Matrix for a region where both $E_c(z)$ and effective mass are constant.

$$\frac{d}{dz}\left(\frac{1}{\gamma(z)}\frac{d\phi}{dz}\right)+\frac{2m_c^*}{\hbar^2}\left[E-\frac{E_t}{\gamma(z)}-E_c\right]\phi(z)=0 \qquad (**)$$

$$\gamma(z)=\frac{m^*(z)}{m_c^*} \qquad E_t=\frac{\hbar^2k_t^2}{2m_c^*} \qquad E=E_p+E_t\;;\; E_p=\frac{\hbar^2k_z^2}{2m_c^*}$$

effective-mass in contacts. $\quad$ in contacts

we search solutions of that equation such that

$$u_1(0)=0 \qquad u_1'(0)=1$$

and

$$u_2(0)=1 \qquad u_2'(0)=0$$

where the prime denotes first derivative with respect to space. The solutions $u_1(z)$, $u_2(z)$ are linearly independent (their Wronskian is unity). A general solution of the equation $(**)$ above can be written as

$$\phi(z)=A_1\,u_1(z)+A_2\,u_2(z)$$

$$\phi(0)=A_2$$

$$\phi'(0)=A_1$$

The transfer matrix is defined as follows

$$\begin{bmatrix}\frac{\phi'(L)}{\gamma}\\ \phi(L)\end{bmatrix}=w\begin{bmatrix}\frac{\phi'(0_+)}{\gamma}\\ \phi(0_+)\end{bmatrix}$$

$$\Longrightarrow\qquad w=\begin{bmatrix}u_1'(L) & \frac{u_2'(L)}{\gamma}\\ \gamma u_1(L) & u_2(L)\end{bmatrix}$$

Note $\boxed{\det w = 1}$ (remember w is independent of z)

The explicit forms for $u_{1,2}(z)$ are the following

$\boxed{\text{Case a}}$ If $E > \frac{E_t}{\gamma} + E_c$

$$u_1(z) = \frac{\sin \beta z}{\beta}$$

$$u_2(z) = \cos \beta z$$

effective mass in region of interest.

where

$$\boxed{\beta^2 = \frac{2m^*}{\hbar^2}\left[E - \frac{E_t}{\gamma} - E_c\right]}$$

$\boxed{\text{case b}}$ If $E < \frac{E_t}{\gamma} + E_c$

$$u_1(z) = \frac{\sinh(Kz)}{K}$$

$$u_2(z) = \cosh(Kz)$$

where

$$\boxed{K^2 = \frac{2m^*}{\hbar^2}\left[\frac{E_t}{\gamma} + E_c - E\right]}$$

$$-\frac{\hbar^2}{2m^*(z)}\frac{\partial^2\psi}{\partial x^2}-\frac{\hbar^2}{2m^*(z)}\frac{\partial^2\psi}{\partial y^2}-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m^*(z)}\frac{\partial\psi}{\partial z}\right]$$

$$+E_c(z)\psi=E\psi$$

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

$$\psi(x,y,z)=\phi(z)e^{i\vec{k}_t\cdot\vec{r}}$$

$$\Downarrow$$

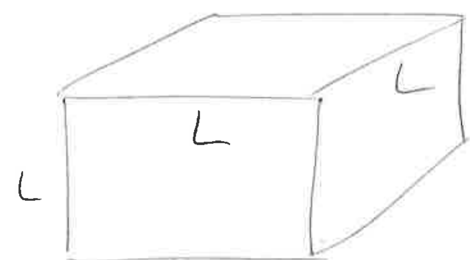
$$\frac{d}{dz}\left[\frac{1}{\gamma(z)}\frac{d\phi}{dz}\right]+\frac{2m_c^*}{\hbar^2}\left\{E_p+E_t\left[1-\gamma^{-1}(z)\right]-E_c(z)\right\}\phi(z)=0$$

$$\gamma(z)=m^*(z)/m_c^*$$

$$\boxed{E_t=\frac{\hbar^2k_t^2}{2m_c^*}\qquad E_p=\frac{\hbar^2k_z^2}{2m_c^*}}$$

$\boxed{\text{In the contacts}}$

Density of States



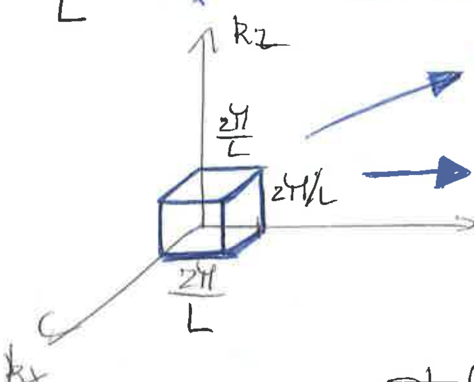
Bloch Theorem

$\psi=e^{ikx}u(x)$ $\quad \psi(x+L)=\psi(x)$

$\phi(x)=Ae^{ikx}+Be^{-ikx}$ $\quad$ Periodic B.C. $\quad$ envelope function is solution of effective mass equation above.

$\longrightarrow$ $k_x=\frac{2n\pi}{L}$ $\quad n_x=0,\pm1,$ $\quad$ (Same for $k_y, k_z = n_y, n_z \frac{2\pi}{L}$) $\boxed{n_y, n_z = 0, \pm1, \pm2}$

$\longrightarrow$



1 state in $\left(\frac{2\pi}{L}\right)^3$

$\frac{d^3\vec{k}}{\left(\frac{2\pi}{L}\right)^3}$ in volume $d^3\vec{k}$

$\longrightarrow$ If spin is taken into account

Density of States $\triangleq 2\frac{L^3}{(2\pi)^3}d^3\vec{k}$

for spin

The total charge density at any point z inside the device is then obtained by adding the total charge density associated with the two oppositely flowing currents. For the particles impinging from the left, we have a total charge density given by

$$n^{l-r}(z) = \frac{1}{4\pi^3}\int d^3k \, |\psi_k^{l-r}(z)|^2 f(E_k)$$

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

is the Fermi-Dirac factor and $\begin{cases} E_k = E_c(0) + \dfrac{\hbar^2k^2}{2m^*} \\ k^2 = k_x^2 + k_y^2 + k_z^2 \end{cases}$

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

Note ψ_k^{l-r} 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 Schroedinger equation. The wavefunction can then be removed from the integration over transverse momentum,

$$n^{l-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} |\psi_{k_BT}^{l-r}(z)|^2 \int_0^{+\infty} \frac{dk_t\, k_t}{\pi}\left[\exp\left(\left(E_c(0) - E_F + \frac{\hbar^2}{2m^*}(k_z^2+k_t^2)\right)/k_BT\right)+1\right]^{-1}$$

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

$$n^{l-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} |\psi_{k_BT}^{l-r}(z)|^2 \, \sigma^{l-r}(k_z) \qquad (**)$$

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

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

$$|\psi_{k_BT}^{l-r}(z)|^2 \rightarrow |\psi_{k_BT}^{r-l}(z)|^2$$

$$\sigma^{l-r}(k_z) \rightarrow \sigma^{r-l}(k_z) \rightarrow \sigma^{l-r} = \sigma^{r-l}$$

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

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18. On page 34 of the notes, it was shown that

$$n^{l-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} \left|\psi^{l-r}_{k_BT}(z)\right|^2 \int_0^{\infty} \frac{k_t\,dk_t}{\pi} \left[\exp\left[\left\{E_c(0) - E_F + \frac{\hbar^2}{2m^*}(k_z^2 + k_t^2)\right\}/k_BT\right] + 1\right]^{-1}$$

Perform the integration over k_t and show ~~that~~

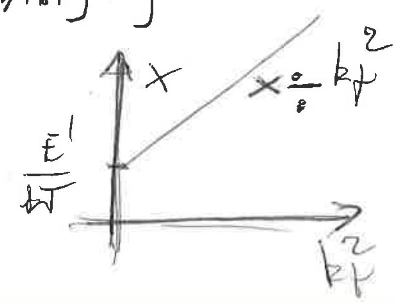
$$n^{l-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} \left|\psi^{l-r}_{k_BT}(z)\right|^2 \sigma^{l-r}(k_z)$$

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

$$\sigma^{l-r}(k_z) = \int_0^{\infty} \frac{dk_t\,k_t}{\pi}\left[\exp\left[\left(E_c(0) - E_f + \frac{\hbar^2}{2m^*}(k_z^2 + k_t^2)\right)/k_BT\right] + 1\right]^{-1}$$

$$= \int_0^{\infty} \frac{dk_t^2}{2\pi}\left[\exp\left(E' + \frac{\hbar^2}{2m^*}k_t^2\right)/k_T + 1\right]^{-1}$$

$$\left(E' = E_c(0) - E_f + \frac{\hbar^2 k_z^2}{2m^*}\right)$$



$$= \frac{2m^* k_BT}{\hbar^2} \int^{\infty} \frac{dx}{2\pi(1+e^x)} \qquad \left(x = \frac{\frac{\hbar^2}{2m^*}k_t^2 + E'}{k_BT}\right)$$

$$= \frac{m^* k_BT}{\hbar^2 \pi} \int_{E'/k_BT}^{\infty} \frac{dx}{1+e^x}$$

$$= \frac{m^* k_BT}{\hbar^2 \pi} \int_{E'/k_BT}^{\infty} \frac{e^{-x}}{1+e^{-x}}\,dx = -\frac{m^* k_BT}{\hbar^2 \pi} \int_{E'/k_BT}^{\infty} \frac{d(1+e^{-x})}{1+e^{-x}}$$

$$= -\left(\frac{m^* k_BT}{\hbar^2 \pi}\right)\left[+\ln(1+e^{-x})\right]_{E'/k_BT}^{\infty}$$

$$= \left(\frac{m^* k_BT}{\hbar^2 \pi}\right) \ln\left(1 + e^{-\frac{E'}{k_BT}}\right)$$

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

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The total electron density is then calculated by adding the two previous contributions
$$n(z) = n^{l-r}(z) + n^{r-l}(z).$$

Electrostatic potential. The Poisson equation to be solved written in its more general form is
$$\frac{d}{dz}\left(\varepsilon(z)\frac{d}{dz}\phi(z)\right) = +q\left[N_D^+(z) - N_A^-(z) - n(z) + p(z)\right]$$
In solving that equation, we have to impose the continuity of
$$\phi(z) \text{ and } \varepsilon(z)\frac{d\phi(z)}{dz}$$

Calculation of Current density

$$\boxed{\vec{J} = \frac{\hbar}{2m^* i}\left[\psi^* \vec{D}\psi - \psi \vec{D}\psi^*\right]}$$

x, y components = 0

z component?

$$J^{l-r} = \frac{-q\hbar}{m^*}\int_0^{+\infty}\frac{dk_z(0)}{2\pi}k_z(0)\, T^{l-r}(k_z(0))\underbrace{\int_0^{+\infty}\frac{dk_t}{\pi}k_t f(E_k)}_{= \sigma^{l-r}(k_z(0))}$$

in left contact

! Transmission coefficient. Go back to definition

where $$T^{l-r} = \frac{k_z(L)}{k_z(0)}\left|\psi^{l-r}_{k_z(0),k_T}(L)\right|^2$$

$$\Longrightarrow J^{l-r} = \frac{-q\hbar}{m^*}\int_0^{+\infty}\frac{dk_z(0)}{2\pi}k_z(L)\,T^{l-r}(k_z(0))\,\sigma^{l-r}(k_z(0))$$

Similarly we calculate J^{r-l} associated to the stream of electrons going from right to left. The total current density through the device is then given by
$$\boxed{J = J^{l-r} - J^{r-l}}$$

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).

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

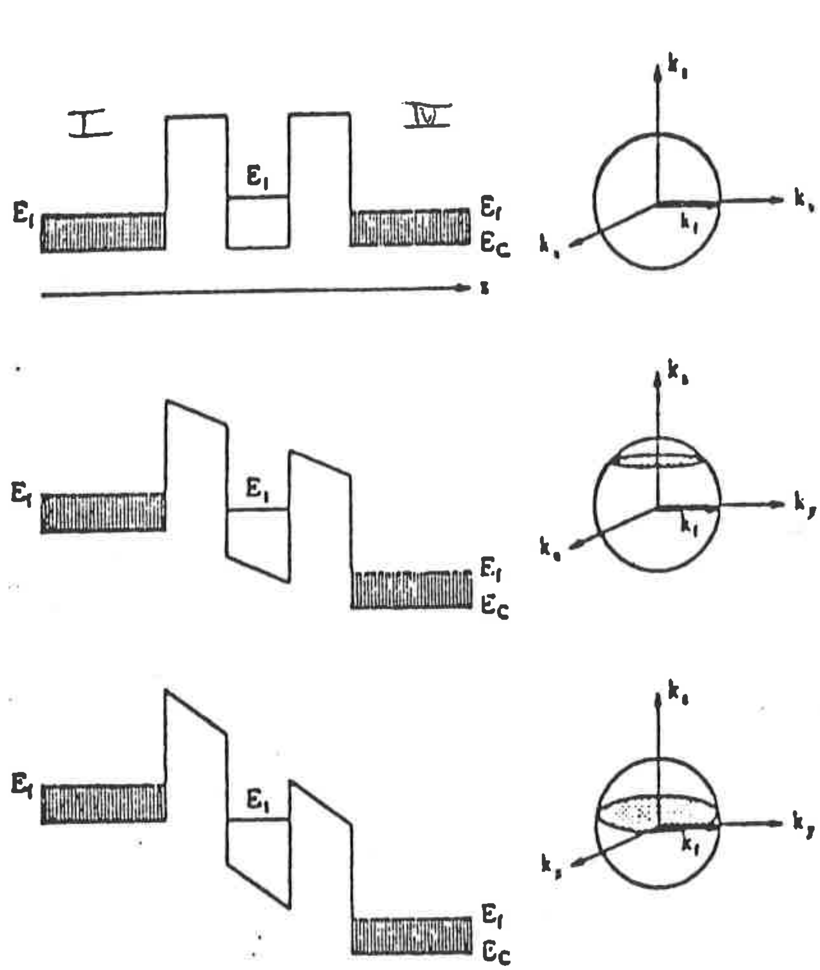
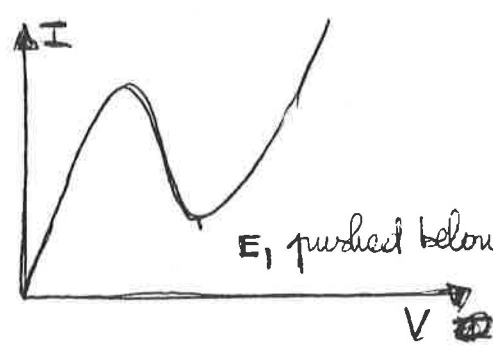
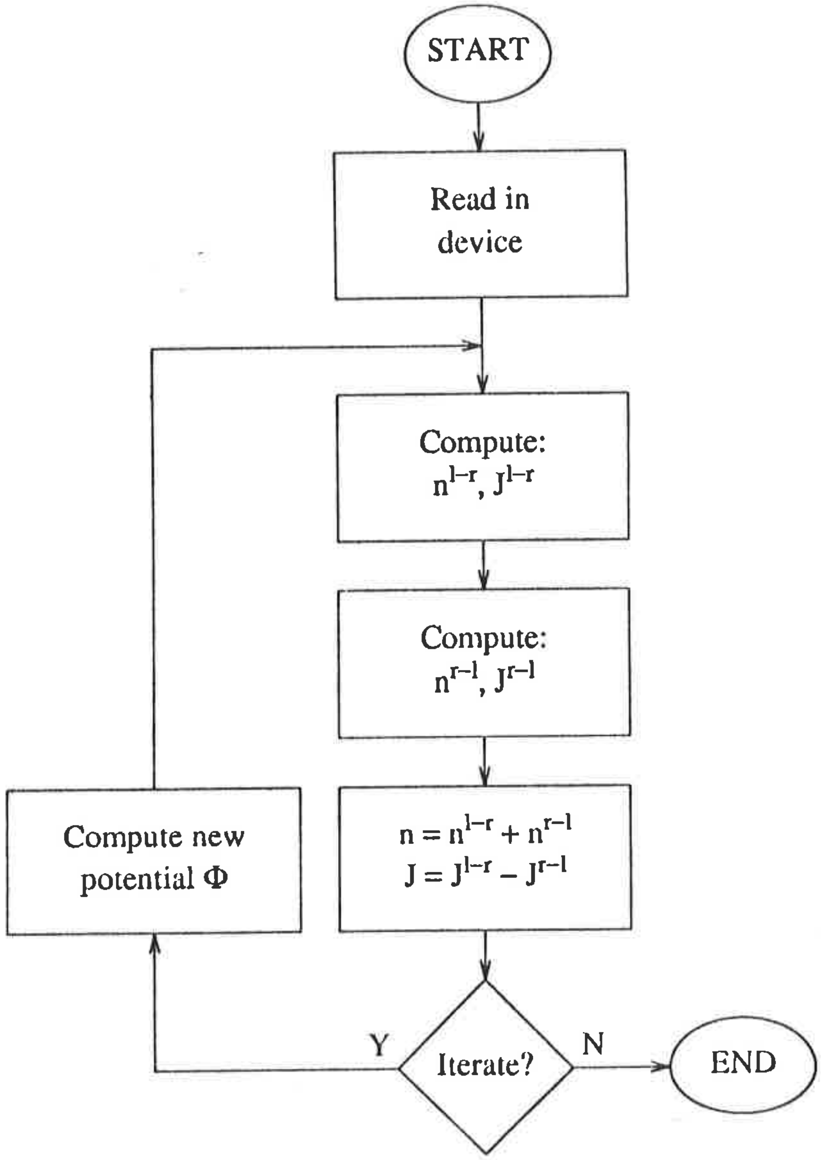


Figure 1.3 Negative differential resistance as a consequence of conservation of transverse momentum.



E_1 pushed below E_c in contact region

Numerical Implementation



SELF CONSISTENT CALCULATIONS

CALCULATION of THE CHARGE DENSITY

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

$$n^{l-r}(z) = \frac{1}{4\pi^3} \int d^3\vec{k} \, | \, \psi_k^{l-r}(z) \, |^2 \, f(E_k)$$

$$E_k = \frac{\hbar^2 k^2}{2m_c^*} + E_C(0)$$

$$n^{l-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} \, | \, \psi_{k_z, k_B T}^{l-r}(z) \, |^2 \int_0^{+\infty} \frac{dk_t k_t}{2\pi} [\exp[(E_C(0) - E_f + \frac{\hbar^2}{2m_c^*}(k_z^2 + k_t^2))/k_B T] + 1]^{-1}.$$

$$n^{l-r}(z) = \int_0^{+\infty} \frac{dk_z}{2\pi} | \, \psi_{k_z, k_B T}^{l-r}(z) \, |^2 \, \sigma^{l-r}(k_z)$$

$$\sigma^{l-r}(k_z) = \frac{m_c^* k_B T}{\pi \hbar^2} \ln[1 + \exp[(E_f - E_C(0) - \hbar^2 k_z^2 / 2m_c^*)/k_B T]]$$

CALCULATION of CURRENT DENSITY

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

$$J^{l-r} = \frac{-q\hbar}{m_c^{*}\pi} \int_0^{+\infty} \frac{dk_z(0)}{2\pi} k_z(0) T^{l-r}(k_z) \int_0^{+\infty} dk_t k_t f(E_k)$$

$$T^{l-r}(k_z) = \frac{k_z(L)}{k_z(0)} \mid \psi^{l-r}_{k_z(0),k_BT}(L) \mid^2$$

$$J^{l-r} = \frac{-q\hbar}{m_c^{*}} \int_0^{+\infty} \frac{dk_z}{2\pi} k_z T^{l-r}(k_z)\, \sigma^{l-r}(k_z)$$

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

$$J^{r-l} = \frac{-q\hbar}{m_c^{*}} \int_0^{+\infty} \frac{dk_z}{2\pi} k_z\, T^{r-l}(k_z)\, \sigma^{r-l}(k_z)$$

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

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

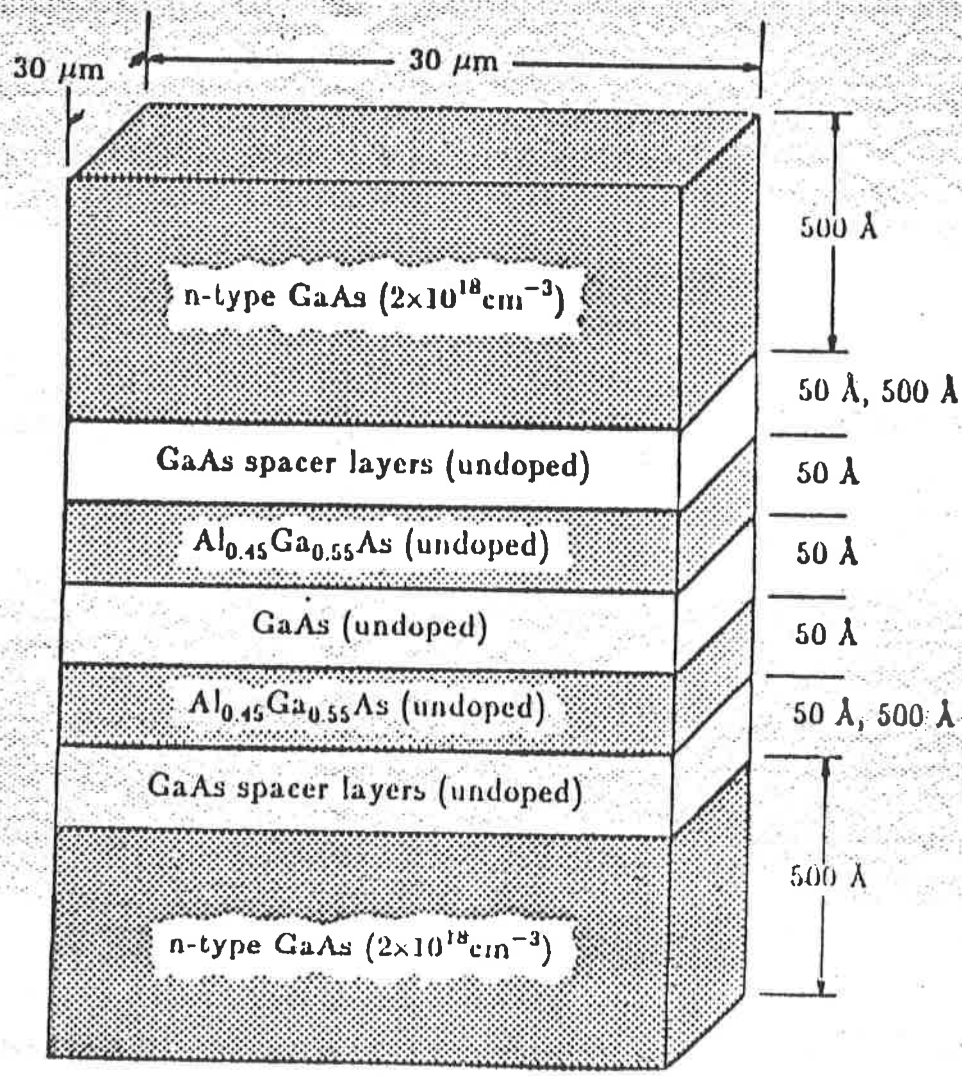
In solving this equation, we have to impose the continuity of

$$\Phi(z) \quad \text{and} \quad \epsilon(z)\frac{d}{dz}\Phi(z)$$

Poisson and Scrödinger equations are then solved iteratively until a self-consistent solution is obtained.

A TYPICAL DEVICE
(RAY and RUDEN)

S. Ray et al. Appl. Phys. Letters Vol. 48(24), pp 1666-1668 (1986)



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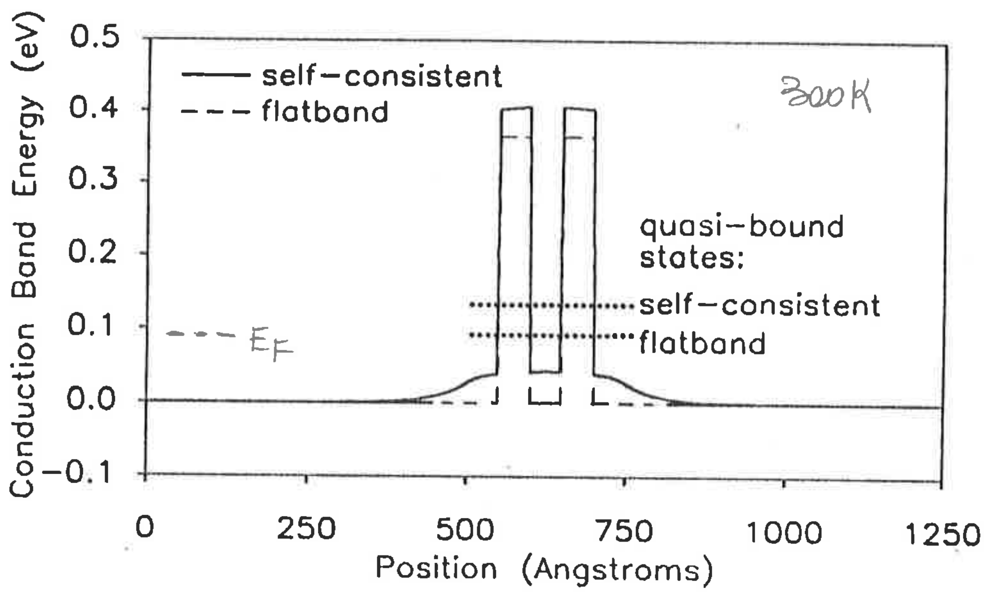
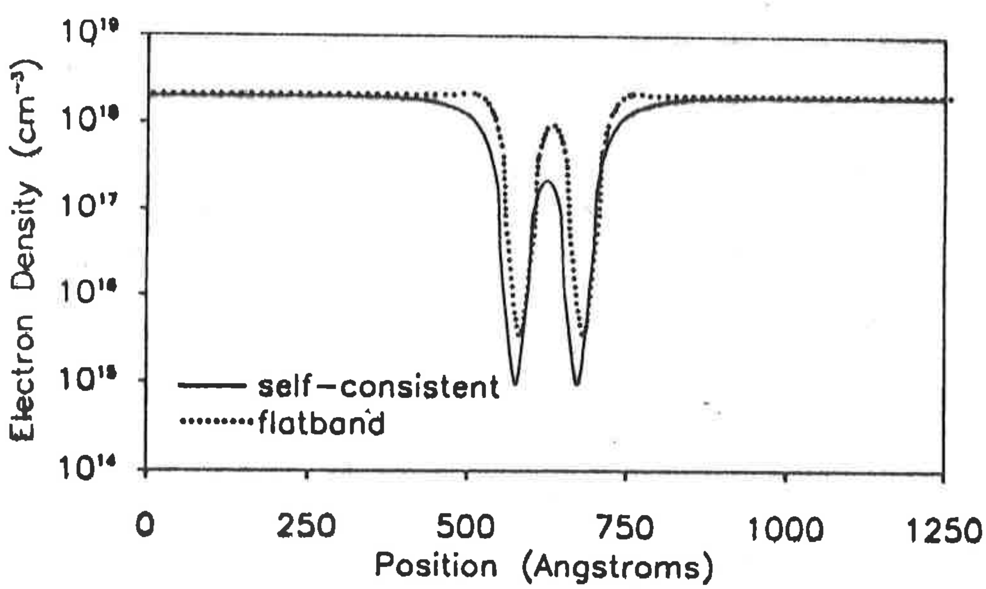
Example Calculations:
50 Å Spacer Layers





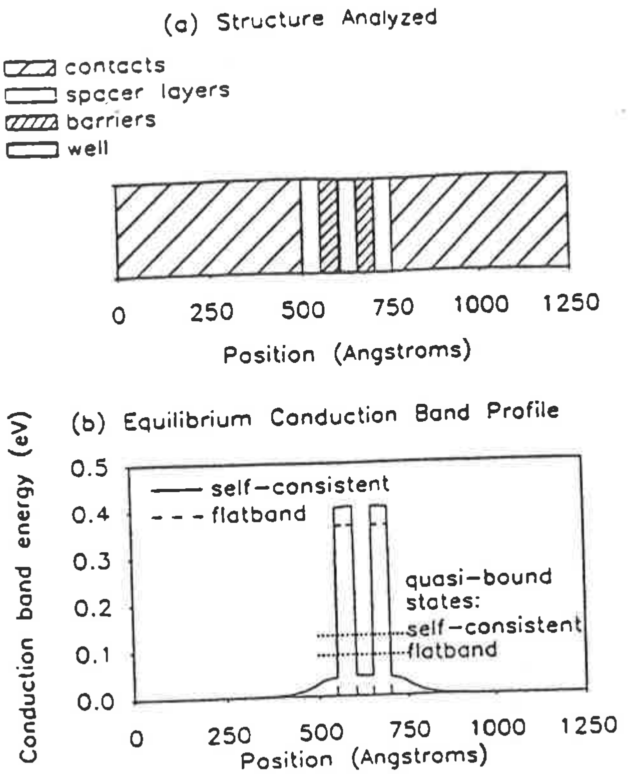


FIG. 1. (a) Structure fabricated by Ray *et al.* (Ref. 4). Contact regions are GaAs doped 2×10^{18} cm^{-3} (Te); spacer regions are undoped GaAs; barriers are undoped $Al_{0.45}Ga_{0.55}As$; and the well is undoped GaAs. (b) Equilibrium conduction-band profiles for self-consistent and flatband calculations.

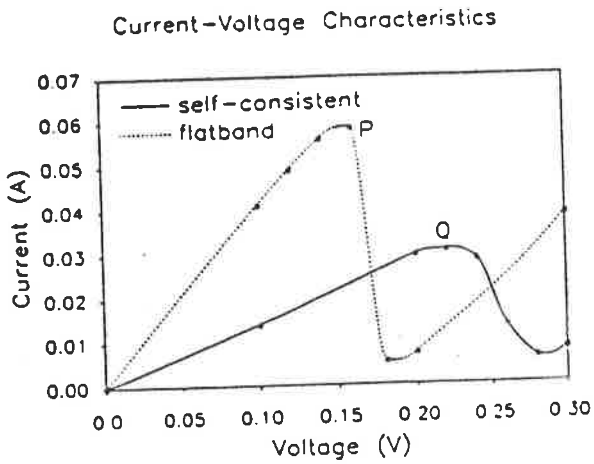


FIG. 2. Current-voltage characteristics (both self-consistent and flatband results) for the structure of Fig. 1, at 300 K. Note that the inclusion of self-consistency has shifted the position of NDR to a higher bias, and broadened the characteristic. In addition, the peak current is reduced for the self-consistent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

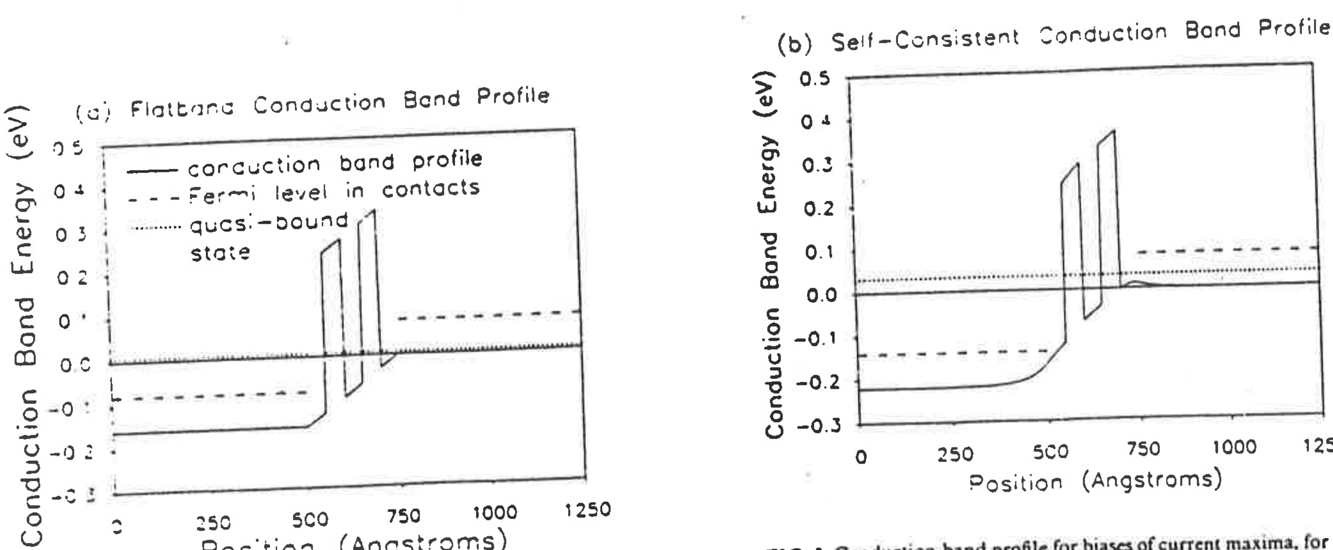
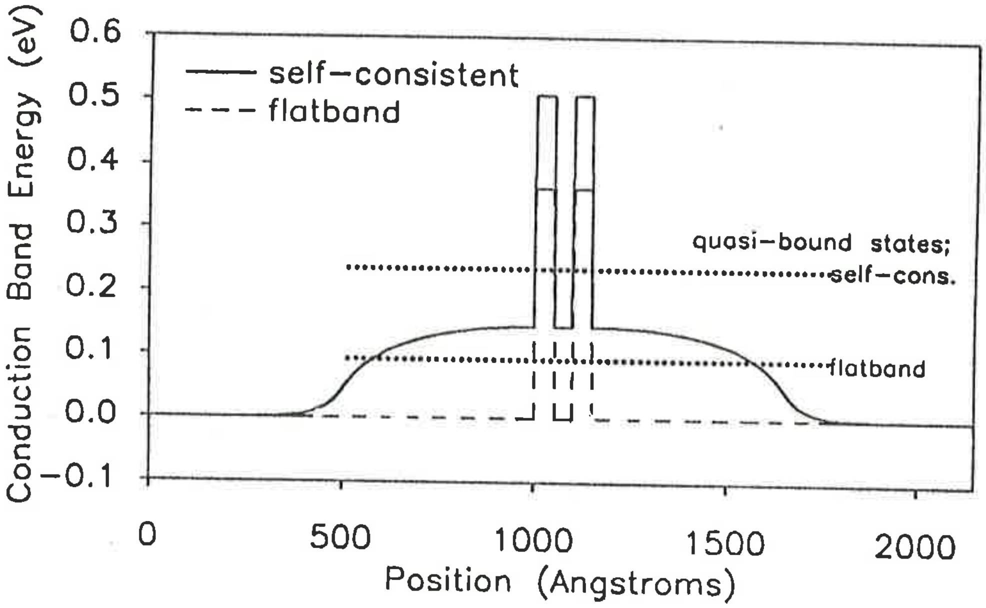
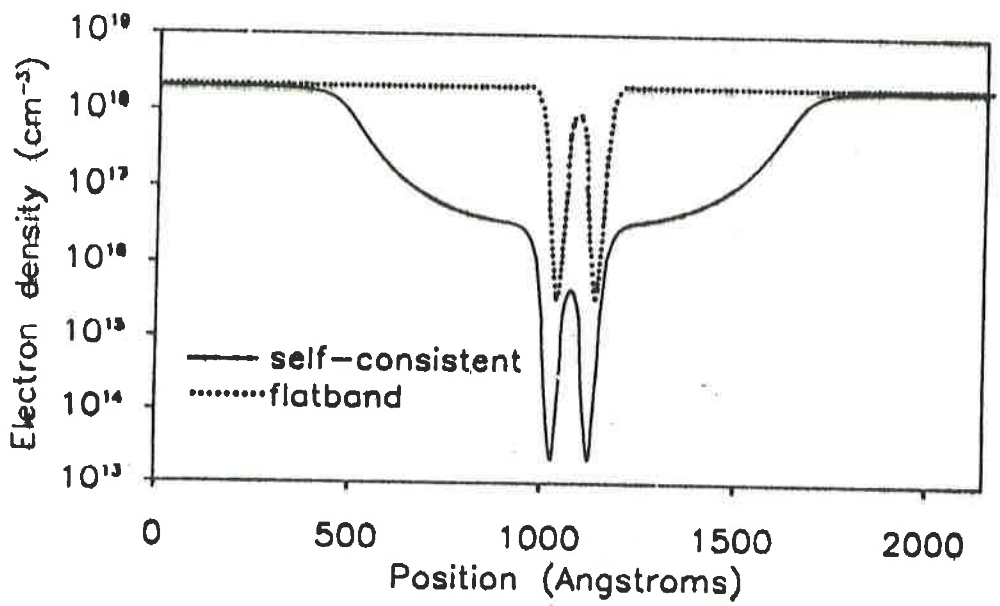


FIG. 3. Conduction-band profile for biases of current maxima, for (a) flatband analysis (point *P* of Fig. 2) and (b) self-consistent analysis (point *Q* of Fig. 2). The level of the quasi-bound state is well above the conduction-band edge in the contact, for the self-consistent case.

Example Calculations:
500 Å Spacer Layers



predict: I_{max} lower; V_{NDR} higher!



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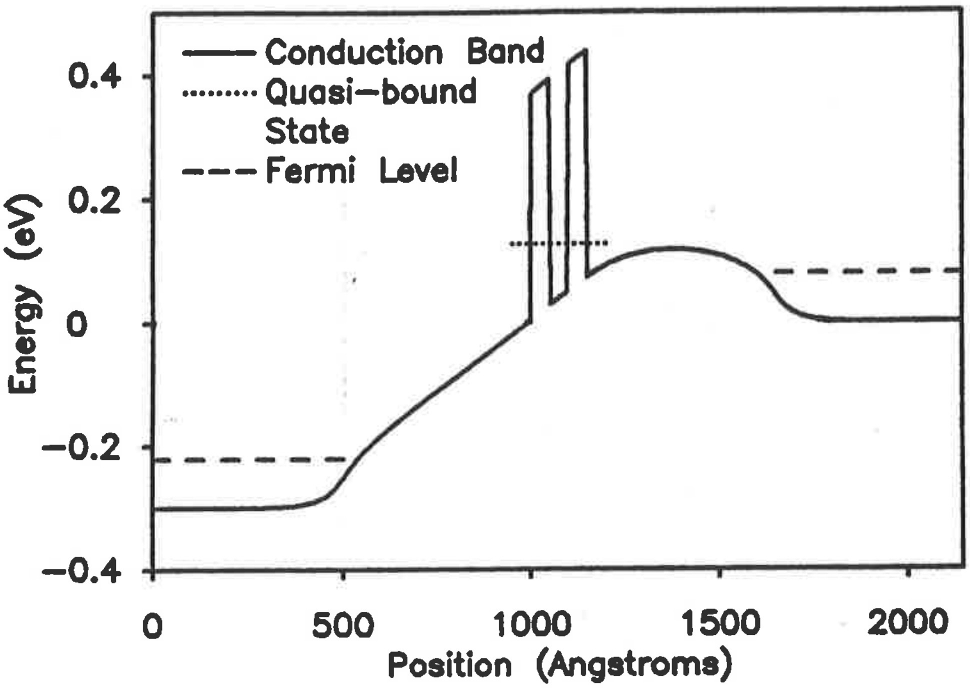

Figure 2.16 SC conduction band profile for the structure with 500 Å spacer layers, at 300° K. The structure is under a bias corresponding to the SC peak current. Any further application of bias causes the quasi-bound state to be "shadowed" by the SC electrostatic potential.

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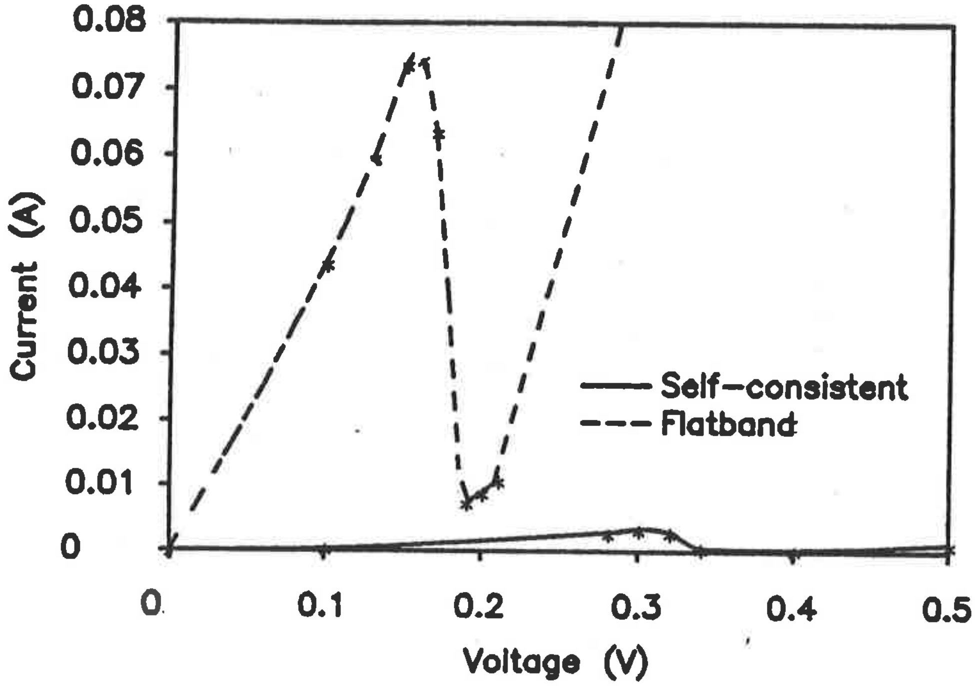

Figure 2.15 Current-voltage characteristics (both SC and NSC calculations) for the structure with 500 Å spacer layers, at 300° K.

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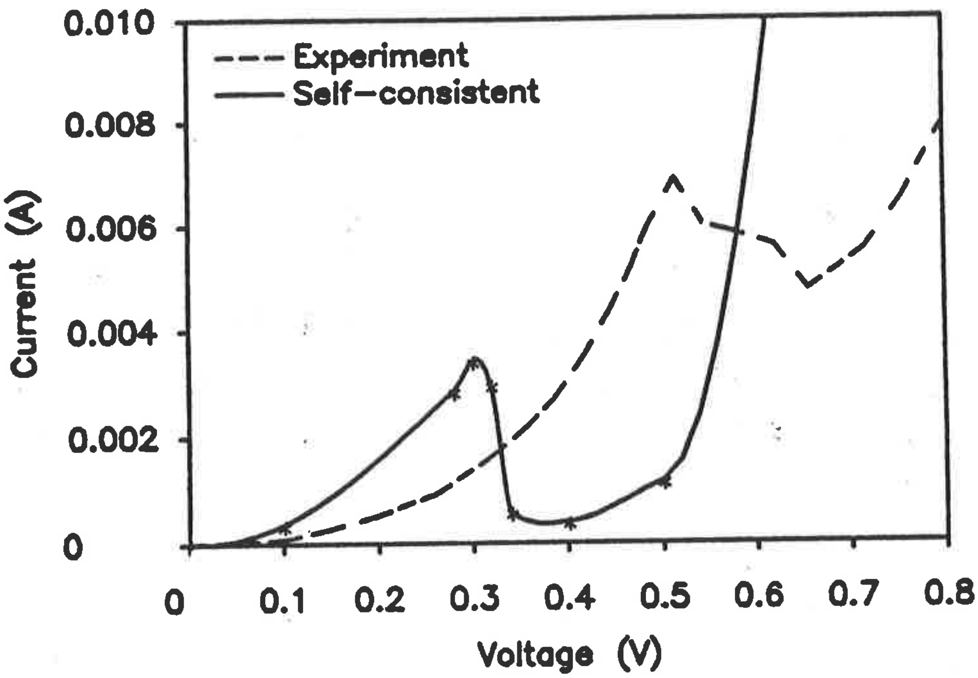

Figure 2.17 Comparison of the SC I-V characteristic and that obtained experimentally by Ray, for the structure with 500 Å spacer layers, at 300° K. Any interpretation of this data should be made with care, since a variety of experimental unknowns can significantly affect results.