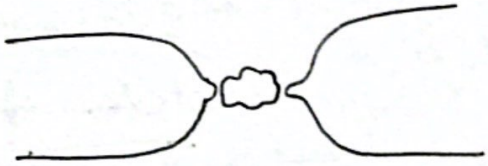
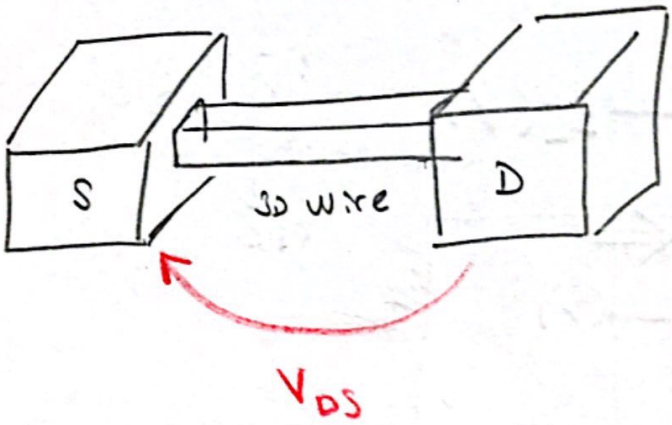
CONDUCTION IN MOLECULAR TRANSISTORS
- A SIMPLE MODEL -

How does conduction happen in this system?



Nanogap + Molecule



3D System

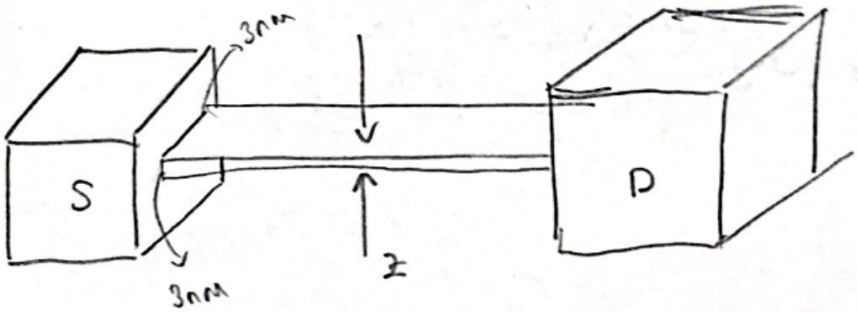
Electrons free to move in all directions of wire

$J_m = q \mu_m . n . \mathcal{E}$ (mobility)

↳ # of charges in a conduction band

↓

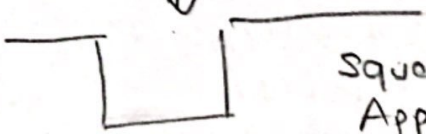
Too Macroscopic!



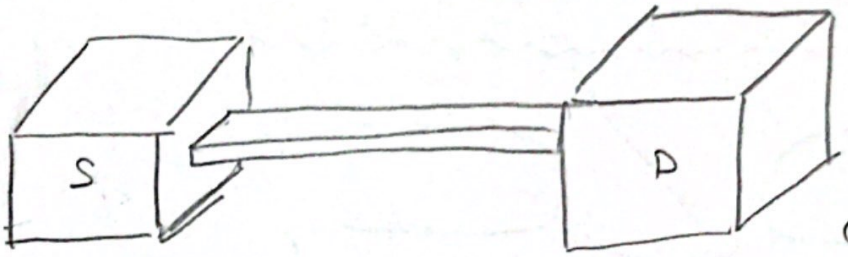
2D Systems

$N_{2D}(E)$ → How Many charges in the wire and how are they distributed?

↓



Square Well Approximation

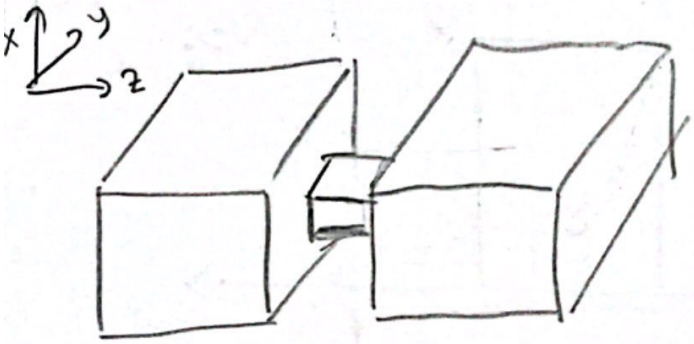


1D System

"Quantum Wire"

Charges can Move in 1 direction

$N_{1D}(E)$? → Bounding Box Model

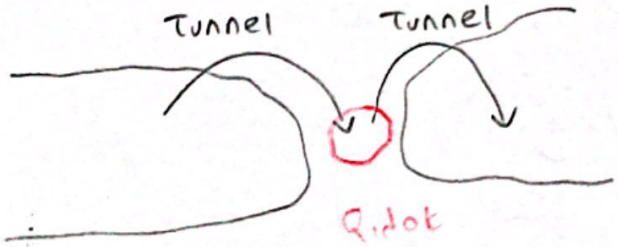


3nM x 3nM x 3nM

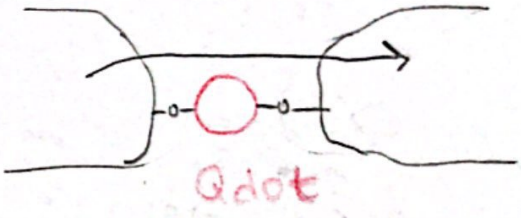
x y z

0D System

"Quantum Dot"



Weak Coupling



Strong Coupling

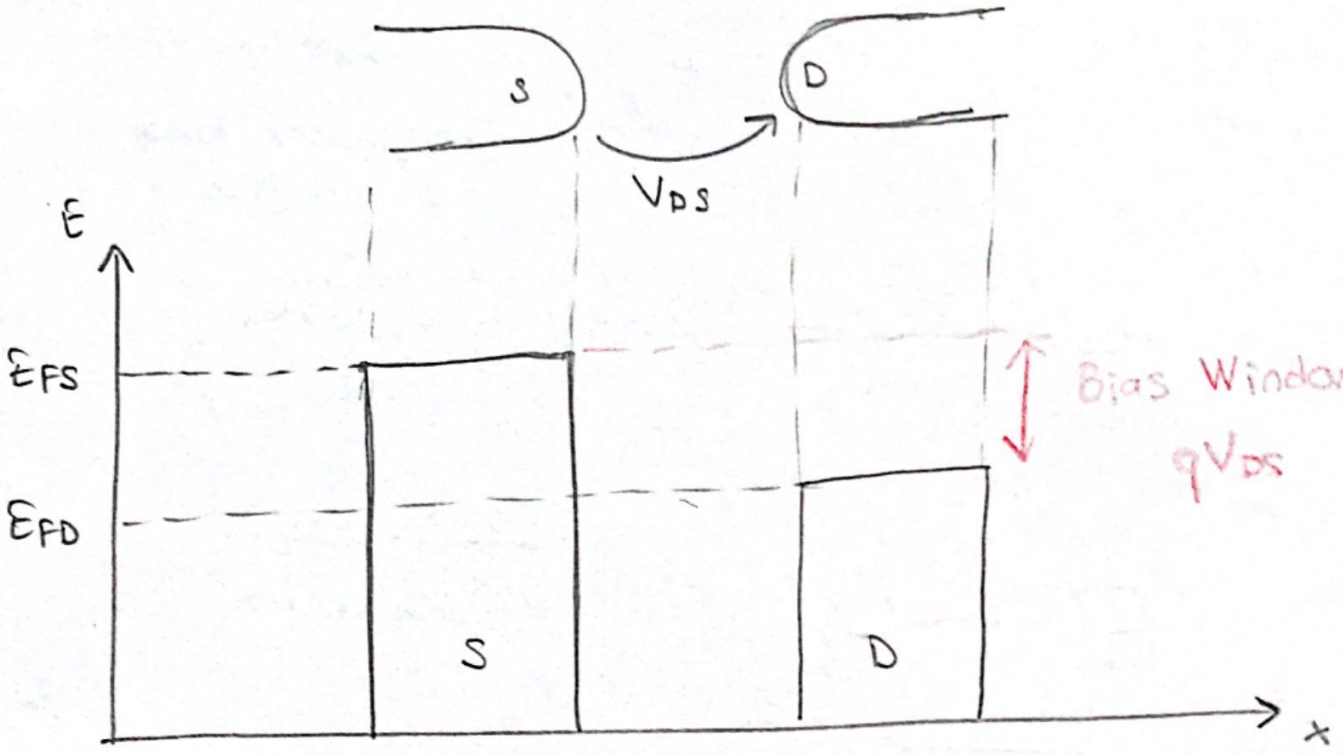
"Molecular Transistors"

* Model for conduction in strongly coupled quantum dots

The flow depends on

- N → # of electrons
- D.O.S → Density of states (# of free states)
- f → Fermi function

Conduction in S.C. Q DOTS



If T=0K

E_{FS} ⇒ Fermi level at source

E_{FD} ⇒ Fermi level at drain

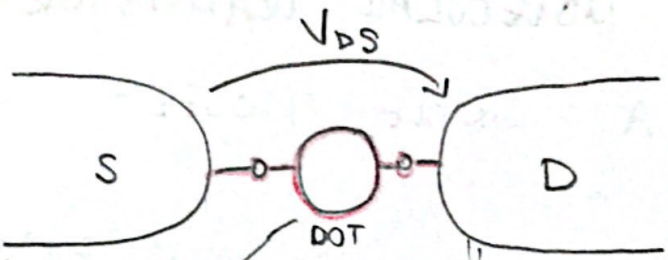
$E > E_{FS}$ → all states are empty

$E < E_{FS}$ → all " " occupied

$$E_{FD} = E_{FS} - qV_{DS}$$

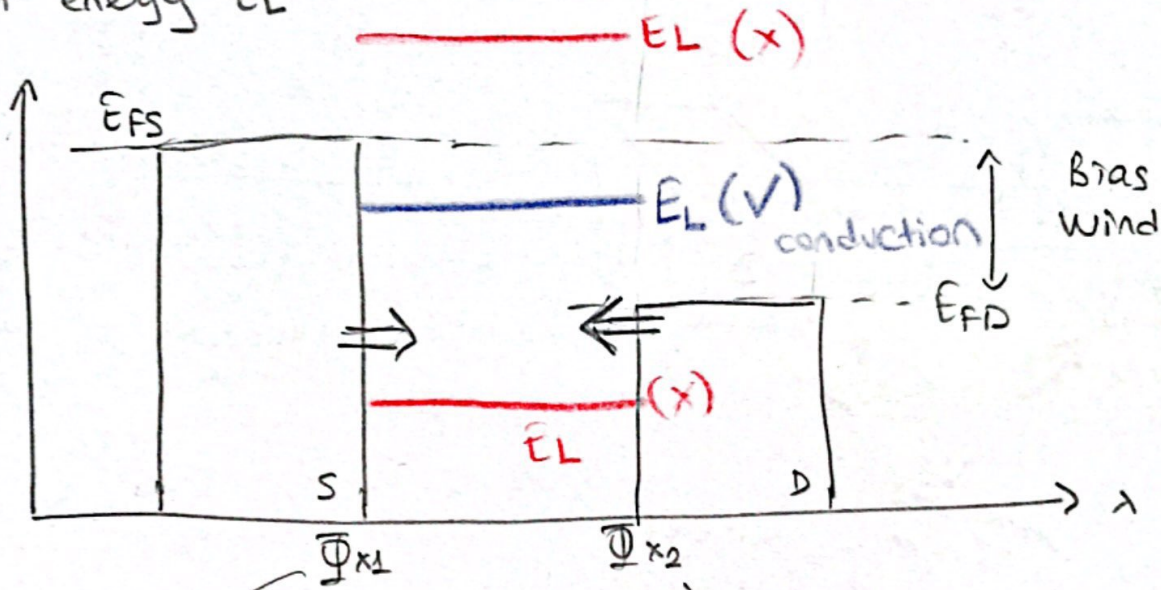
$$f(E, E_{FS}) = \frac{1}{1 + e^{\frac{E - E_{FS}}{kT}}}$$

$$f(E, E_{FD}) = \frac{1}{1 + e^{\frac{E - E_{FD}}{kT}}}$$



The DOT contributes with N electrons $\bar{e}$ at energy E_L

Contributes with discrete level of possible energy states.



$E_{FS} < E_L < E_{FD}$

Φ_{x1}, Φ_{x2} } Fluxes of electrons from electrodes to dot

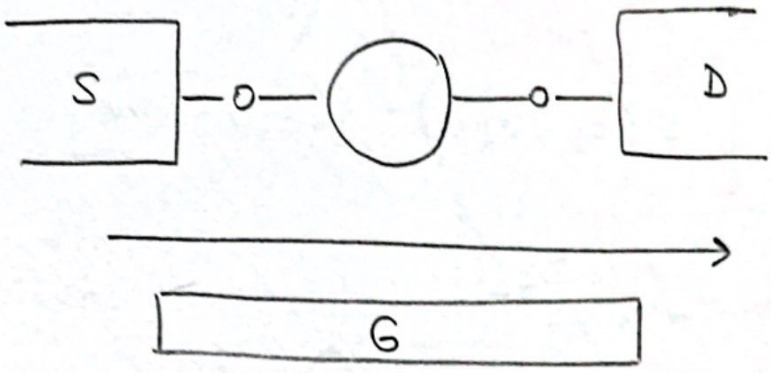
$$\tau_1 = \frac{\hbar}{\gamma_1}$$

$$\tau_2 = \frac{\hbar}{\gamma_2}$$

coupling factor (happiness of electrons :)

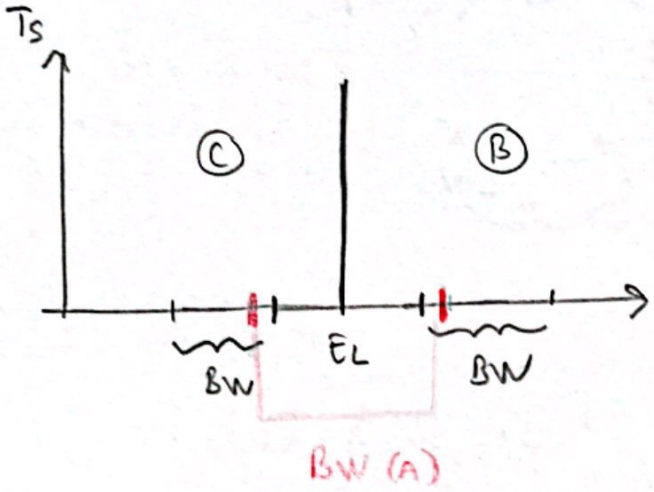
Transfer time bw source & dot (1) drain & dot (2)

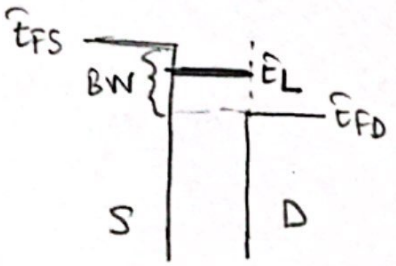
NT Behavior & Characteristic Part 1



$$I_{DS} = \frac{2q}{h} \underbrace{\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}} \left[f(E_L, E_{FS}) - f(E_L - E_{FD}) \right]$$

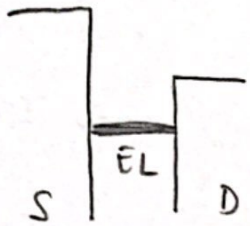
Coupling factor





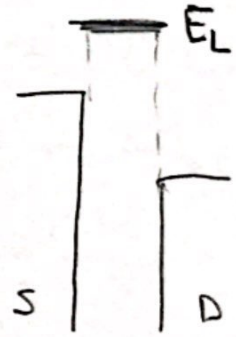
(A)

$I_{DS} > 0$



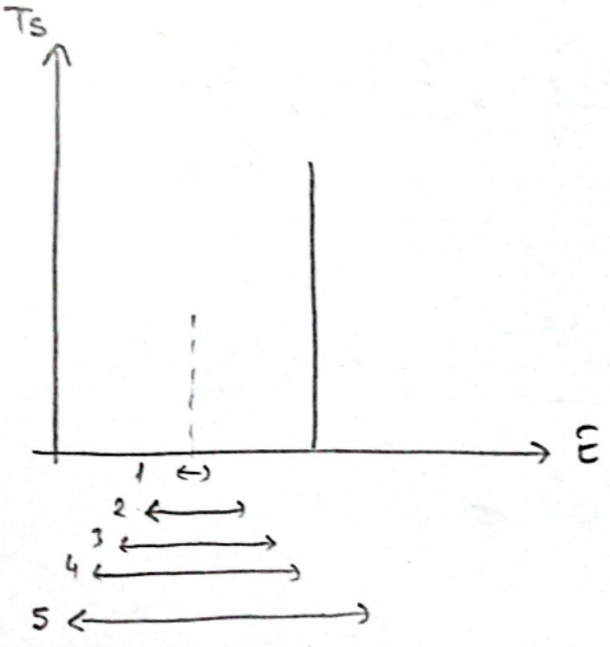
(B)

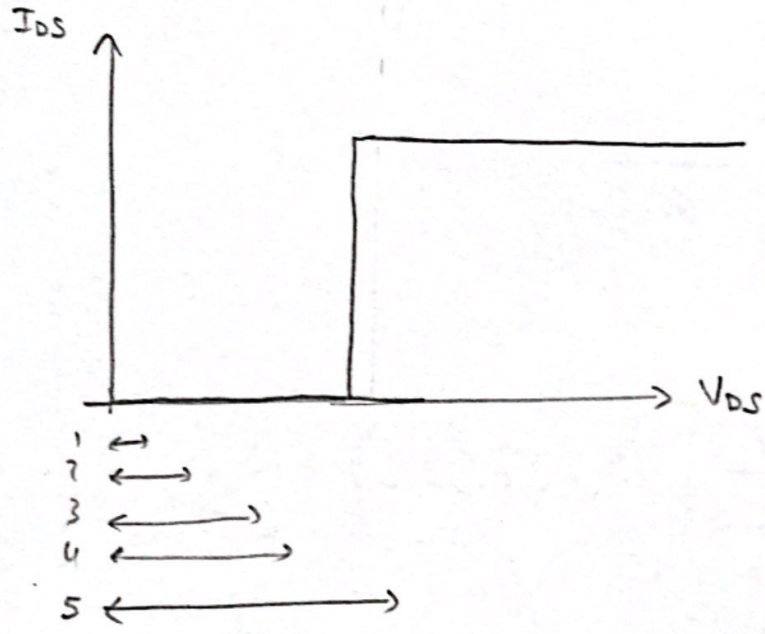
$I_{DS} = 0$



(C)

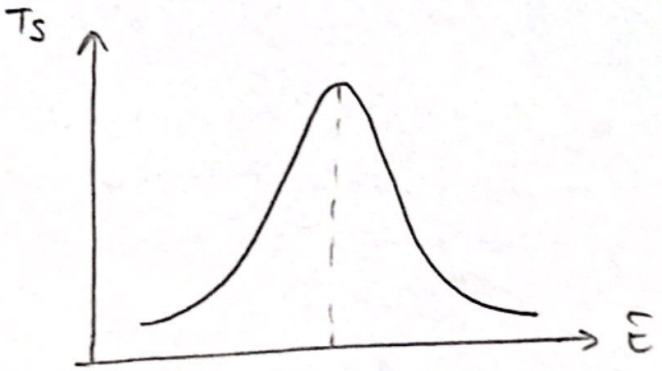
$I_{DS} = 0$





V_{DS} is associated to BW of increasing value.

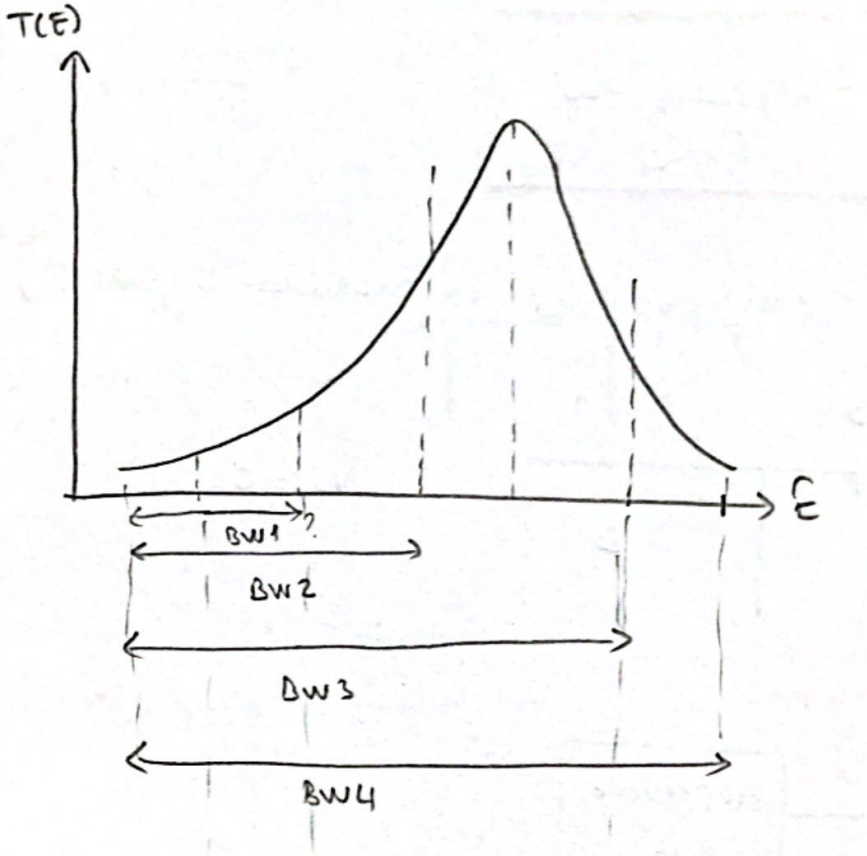
In case of a molecule

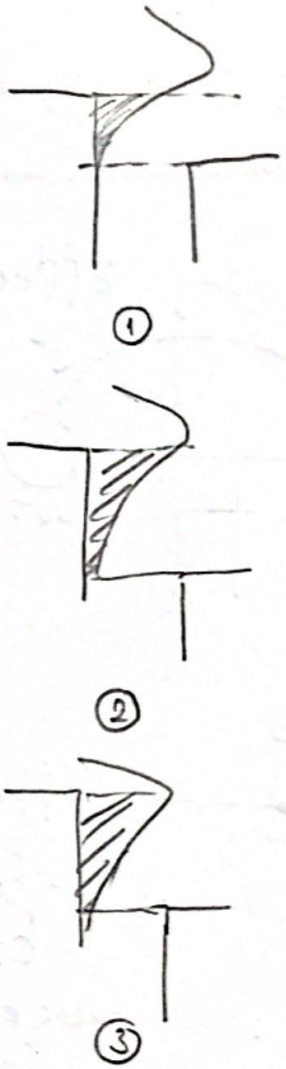


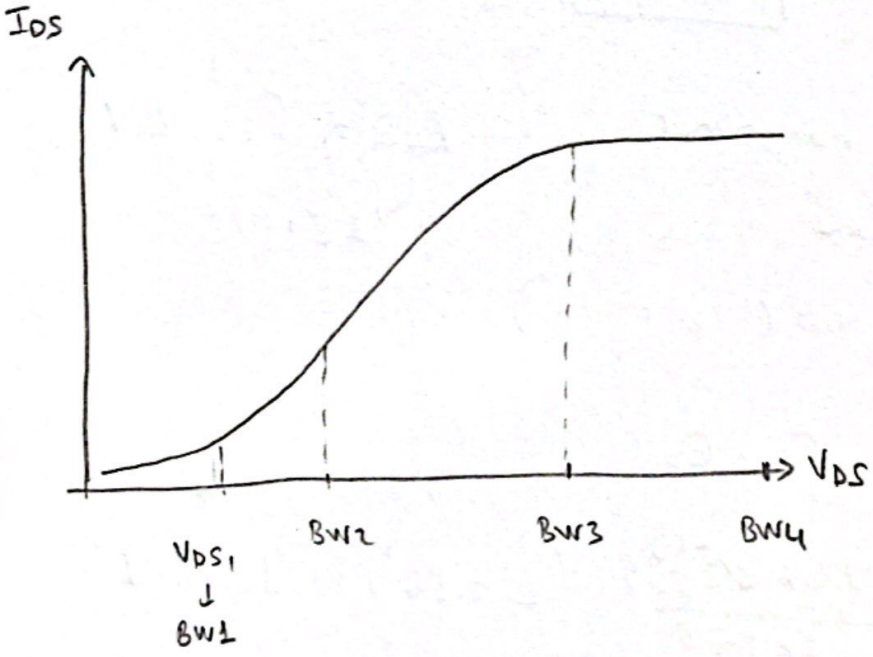
↳ Density of State

$$D(E) = \frac{\Gamma/2\pi}{(E-E_L)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

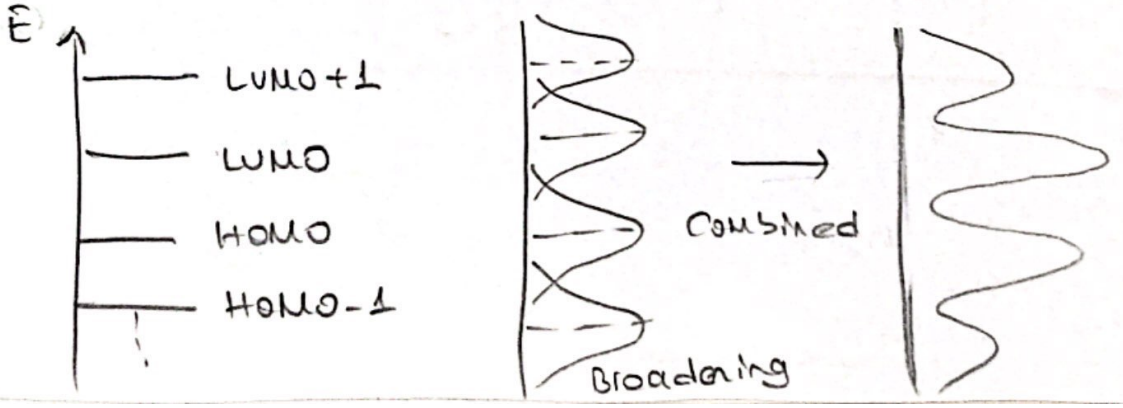
$$I_{DS} = \frac{2q}{\hbar} \int_{-\infty}^{\infty} \underbrace{\frac{\gamma_1 \gamma_2}{\gamma_1+\gamma_2}}_{\text{Transmission Spectrum}} D(E).\left[f(E,E_{FS}) - f(E,E_{FD})\right]$$

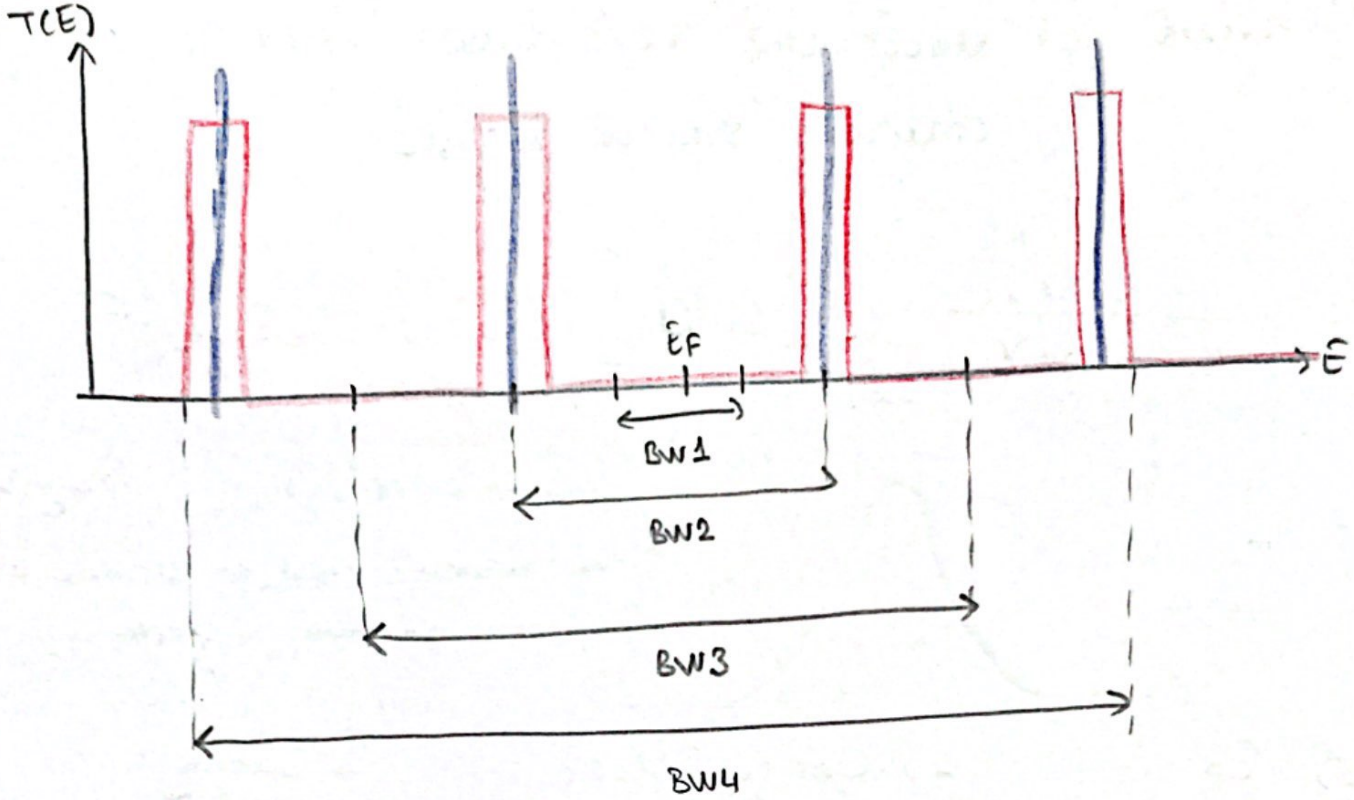


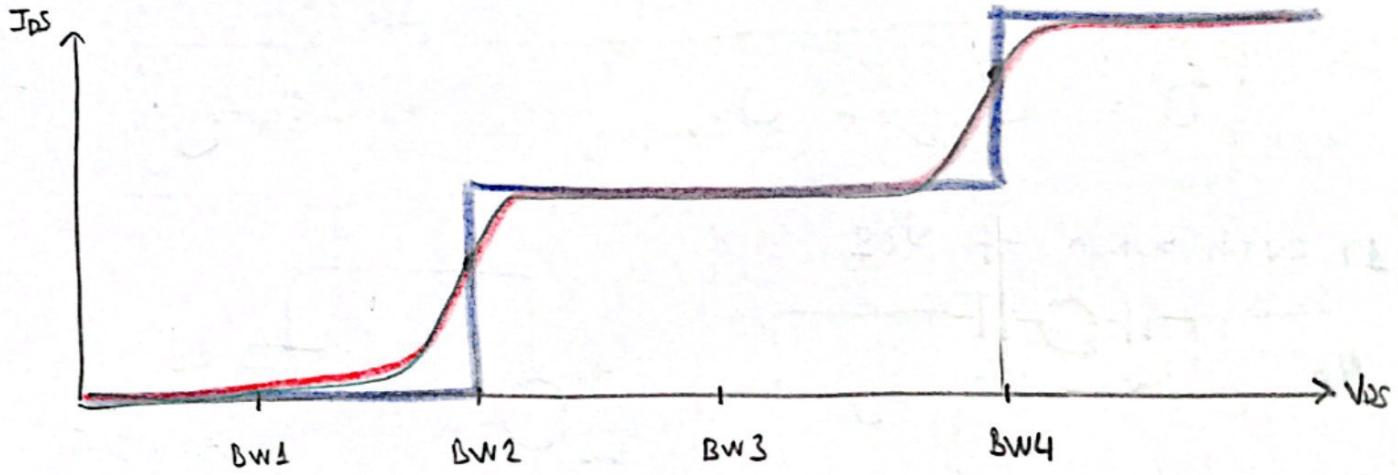




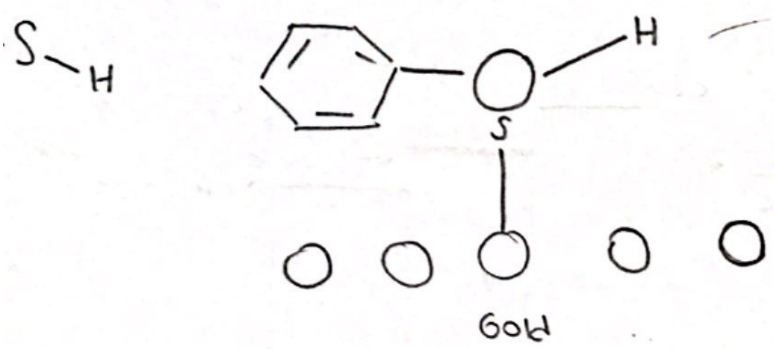
★ In a real Molecule → More than one peak







Dithol - Benzene



MODELING OF MOLECULAR TRANSISTOR PART 2

COMPLETE SIMPLE MODEL

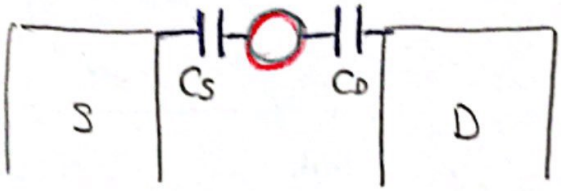
$$I_{DS} = \frac{q}{h}\frac{2\Gamma_1\Gamma_2}{\Gamma_1+\Gamma_2}\int_{-\infty} D_{EL}(E-U)\left[f(E,E_B)-f(E,E_{FD})\right]dE$$

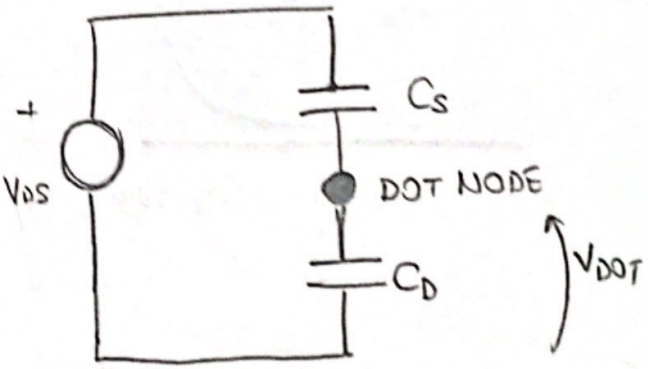
U → generalization for the energy of the system used to model other effects on the system.

1) $E_{F\,DOT}$ 2) Charge Effect 3) Gating

$$U = U_{V_{DS}} + U_{charging\ effect} + U_{Gating}$$

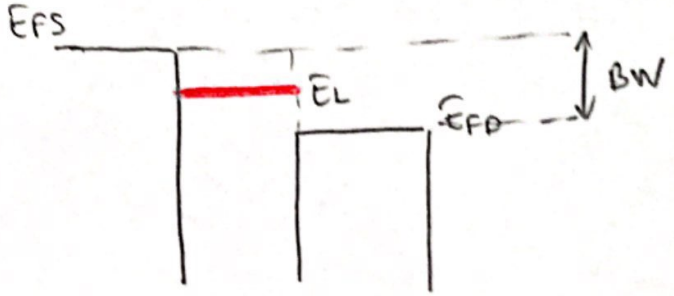
1) contribution of V_{DS}





$$V_{DOT} = V_{DS}\cdot\frac{C_D}{C_D+C_S}$$

If $C_S = C_D \Rightarrow V_{DOT} = V_{DS}\cdot\frac{1}{2}$

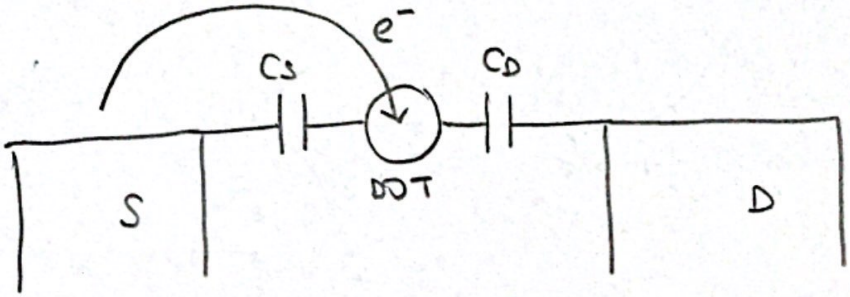


$$E_{FDOT} = E_{FS} - \frac{qV_{DS}}{2}$$

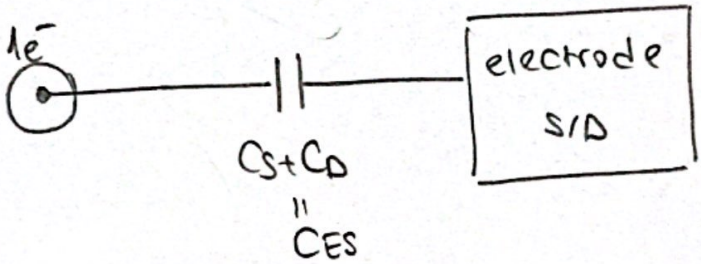
$$E_L = E_{FDOT}$$

$$U_{V_{DS}} = -q V_{DOT} = -q \frac{C_D}{C_S + C_D} \cdot V_{DS}$$

2) Charging Effect (Not observed in standard systems)



$V_{DS} = 0$



→ DOT is a charge container

→ S or D is an electrode

→ Capacitance is the sum (parallel)

$$\Delta Q = C_{ES} \cdot \Delta V$$

↳ 1 é

$$C_{ES} = C_S + C_D$$

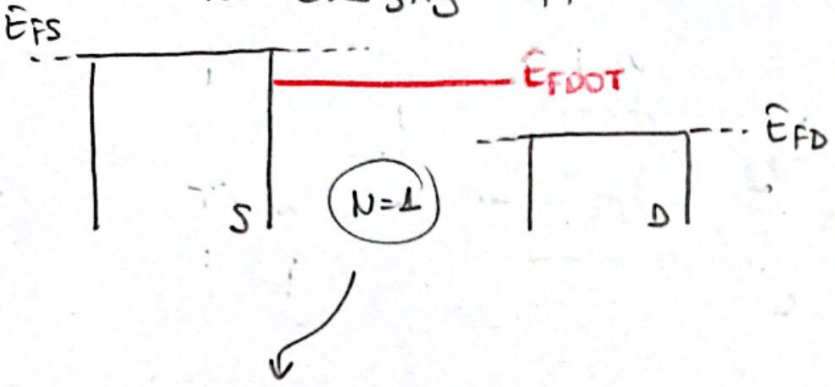
$$\Delta Q = -q$$

$$\Delta V = \frac{-q}{C_{ES}} = \frac{1{,}6 \times 10^{-19}}{1 \times 10^{-18}} = -0{,}16\ V = 160\ mV$$

$$U_{charging\ Effect} = -q\Delta V = \frac{q^2}{C_{ES}} \approx 0{,}16\ eV$$

2.1 Charging Effect when $V_{DS} \neq 0$

No charging Effect (No C.E)



$$N = \frac{2}{\gamma_1 + \gamma_2}\left[\gamma_1 f(E_L, E_{FS}) + \gamma_2 f(E_L, E_{FD})\right]$$

$f(E_L, E_{FS})$ → 1 → occupied states

$f(E_L, E_{FD})$ → 0 → Unoccupied states

if $\gamma_1 = \gamma_2 \Rightarrow N = \frac{2\gamma_1}{2\gamma_1} = 1$,

If C.E is considered

↳ when $1e^-$ Jumps in the channel

↳ U changes 0.16 eV

Self- Consisted field : SCF

$$N = \frac{2}{\gamma_1+\gamma_2} \int_{too}^{\infty} D_{EL}(E-U)\left[\gamma_1 f(E,E_{FS}) + \gamma_2 f(E,E_{FD})\right] dE$$

$$U_{C.E} = U_0 (N - N_0)$$

SCF loop

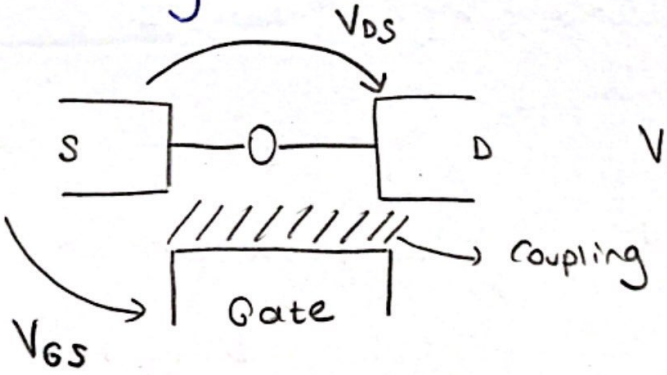
$U_{C.E}$ ↓ charging effect

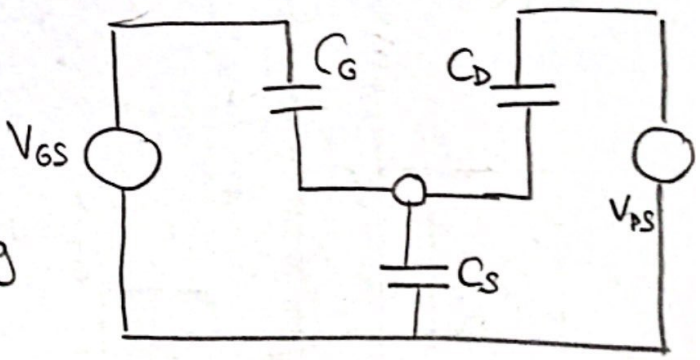
$$U_0 = \frac{q^2}{C_{ES}}$$

N_0 = # of electrons at equilibrium

N = Actual # of electrons

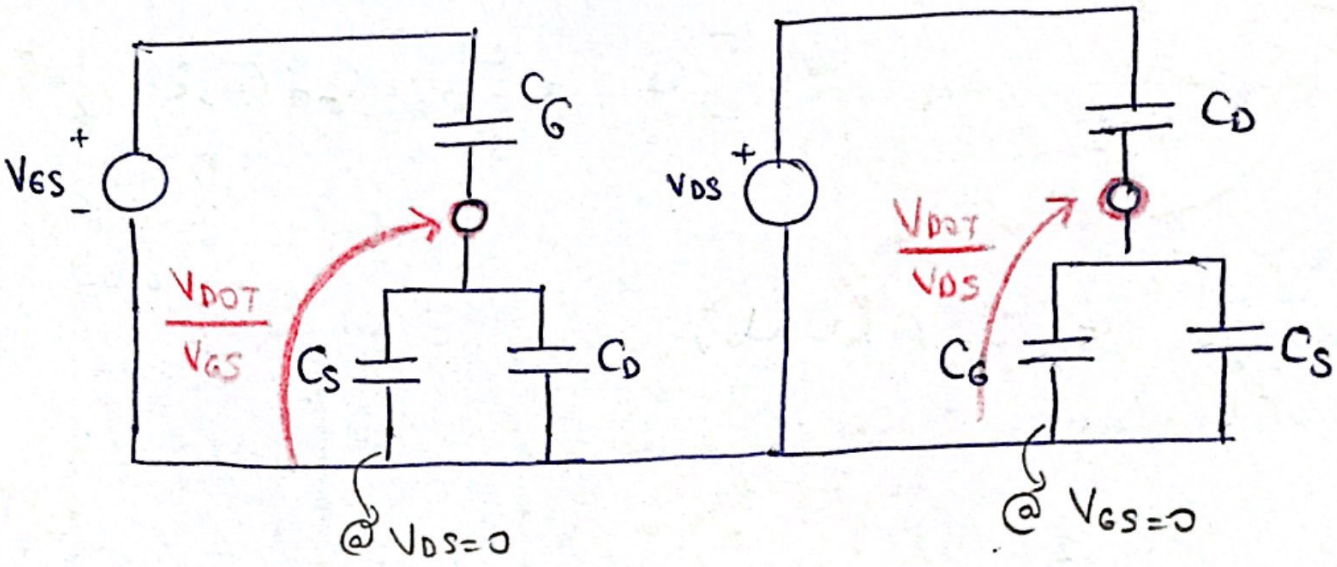
3) Gating





C_6 Models the contact with the gate through a coupling factor

Superposition of Effects

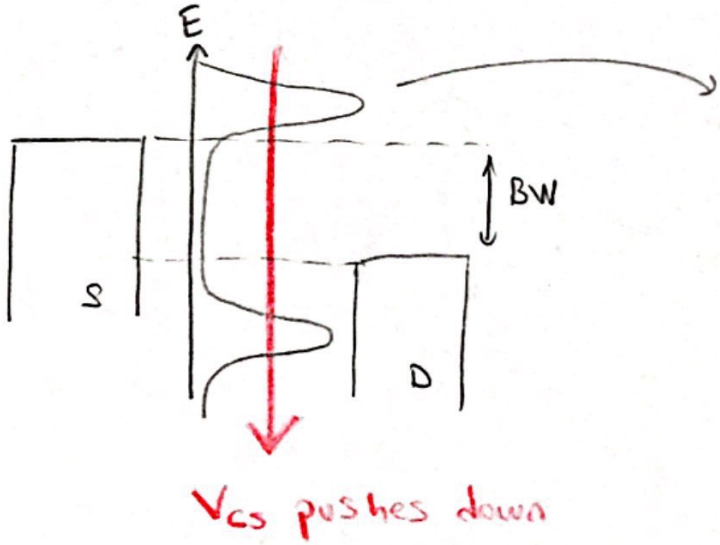


$$U_{V_{GS}} = -q\frac{V_{DOT}}{V_{GS}} = -q\left(V_{GS}\cdot\frac{C_G}{C_G + C_S /\!/ C_D}\right)$$

C_{ES}

$V_{GS}>0$ $U_{V_{GS}}$ ↘ toward lower energies

$V_{GS}<0$ $U_{V_{GS}}$ ↗ toward higher energies



Initially not in BW

V_{GS} pushes down E

↓

↓ peak might enter in BW!!!

$V_{GS}>0$ $U_{V_{GS}}$ ↓

Overall

$$U = U_{VGS} + U_{VDS} + U_{CE}$$

$$U_{VGS} = -q V_{GS} \cdot \frac{C_D}{C_{ES}}$$

$$U_{CE} = -\frac{q^2}{C_{ES}}$$

$$U_{VDS} = -q V_{DS} \cdot \frac{C_D}{C_{ES}}$$

$$C_{ES} = C_G + C_S + C_D$$