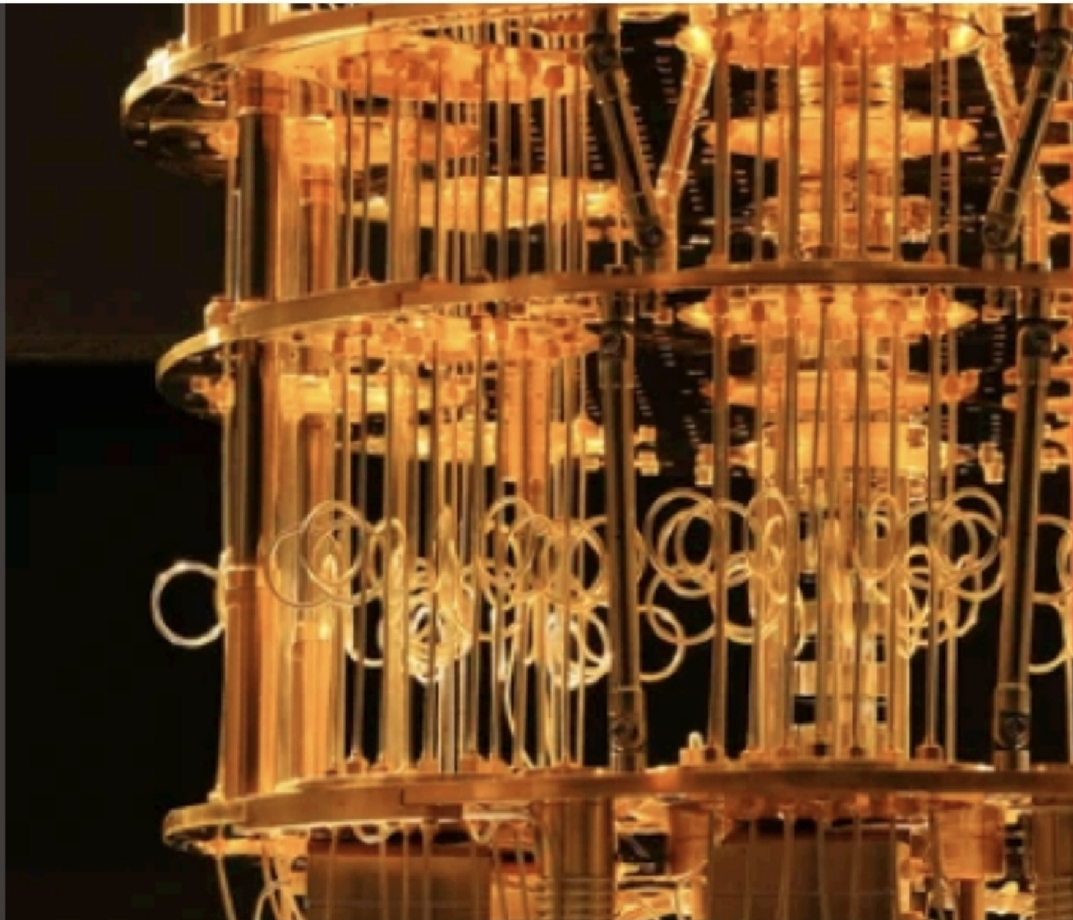


MICRO-435 Quantum and Nanocomputing

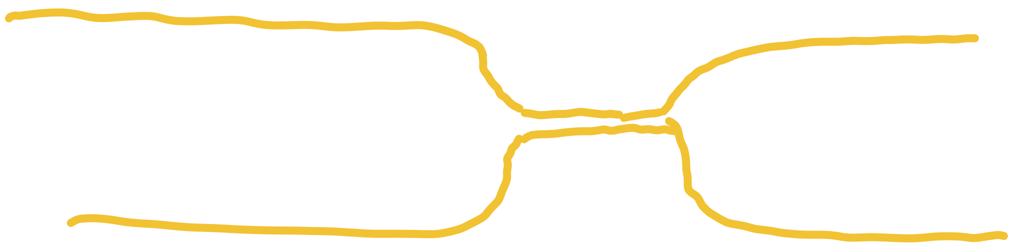
Edoardo Charbon
Mariagrazia Graziano

CONDUCTION IN MOLECULAR TRANSISTORS

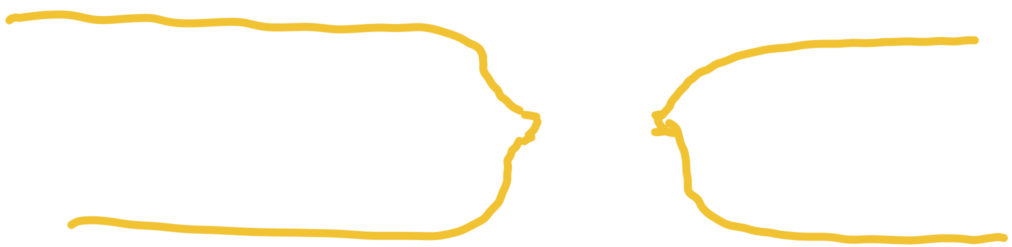
A SIMPLE MODEL

11-12 | 11 | 25

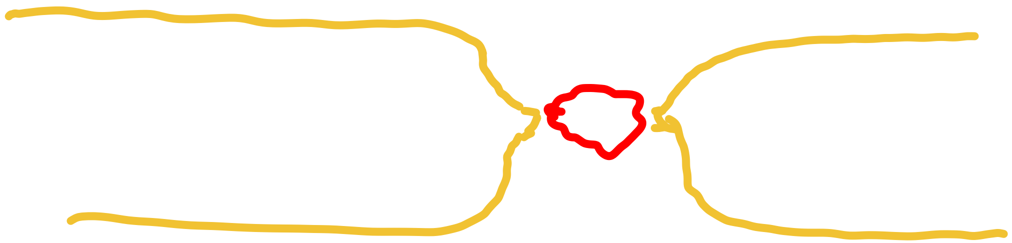
THE REFENCE SYSTEM



NANOWIRE

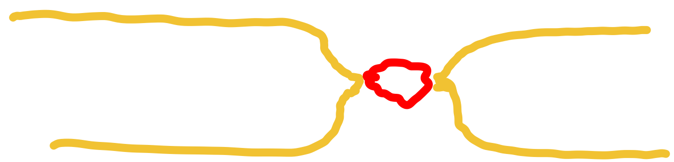


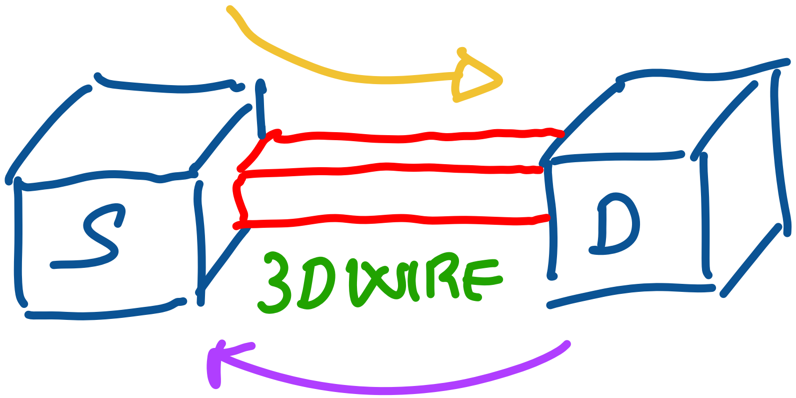
NANOGAP



NANOGAP
+
MOLECULE

HOW DOES CONDUCTION HAPPEN IN THIS SYSTEM?





3D SYSTEM

ELECTRONS FREE TO MOVE IN ALL DIRECTIONS OF WIRE

$V_{DS} \rightarrow \mathcal{E}$ ENERGY

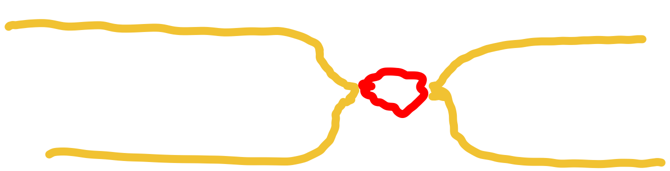
$$J_n = q \mu_n \cdot n \mathcal{E}$$

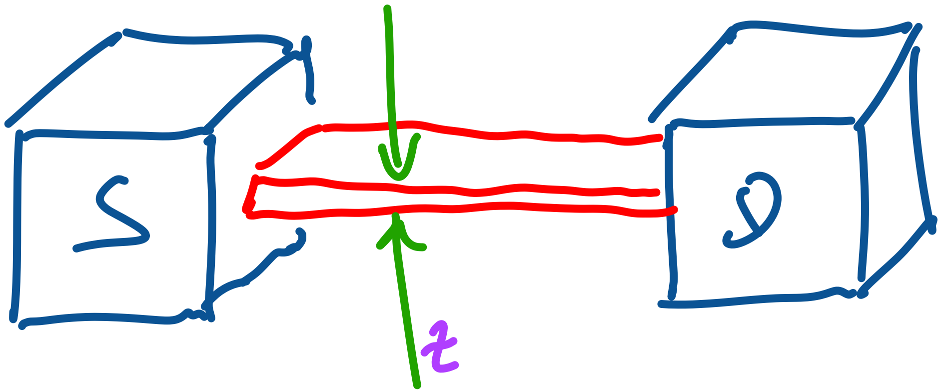
CURRENT IN THE CRISTAL WITH SCATTERING

TOO MACROSCOPIC (↗ J_n)

NUMBER OF CHARGES IN A CONDUCTION BAND (↑ n)

HOW DOES CONDUCTION HAPPEN IN THIS SYSTEM?



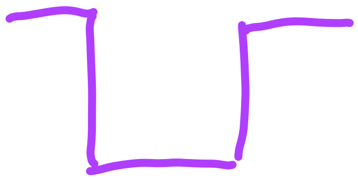


2D SYSTEMS

1 DIRECTION IS CONFINED DUE TO SCALING AT nm SIZE

ELECTRONS ARE FREE IN 2 DIRECTIONS

CONFINED IN 1 DIRECTION

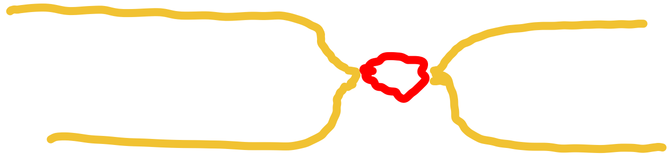


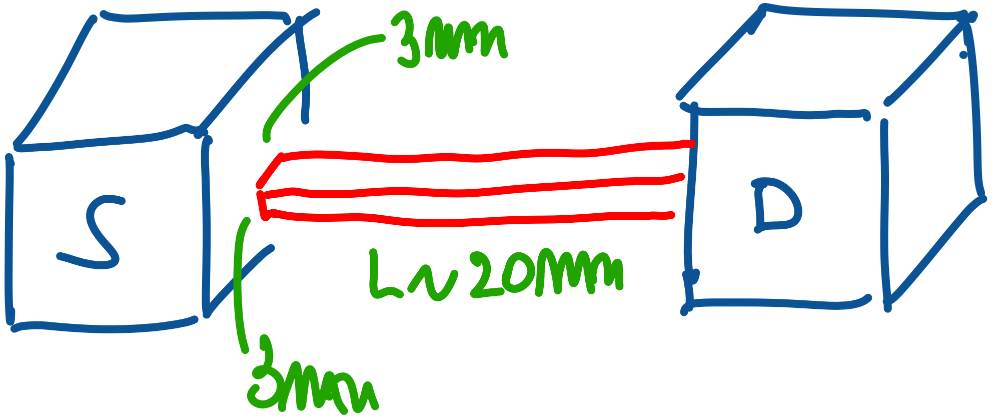
$N_{2D}(E)$ HOW MANY CHARGES IN THE WIRE AND HOW DISTRIBUTED?

⇒ SQUARE WELL APPROXIMATION

TOO MACROSCOPIC

HOW DOES CONDUCTION HAPPEN IN THIS SYSTEM?





1D SYSTEM

QUANTUM WIRE

CHARGES CAN MOVE IN 1 DIRECTION

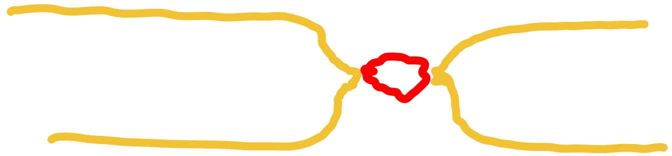
EACH ELECTRON CONTRIBUTES INDIVIDUALLY TO THE CONDUCTION

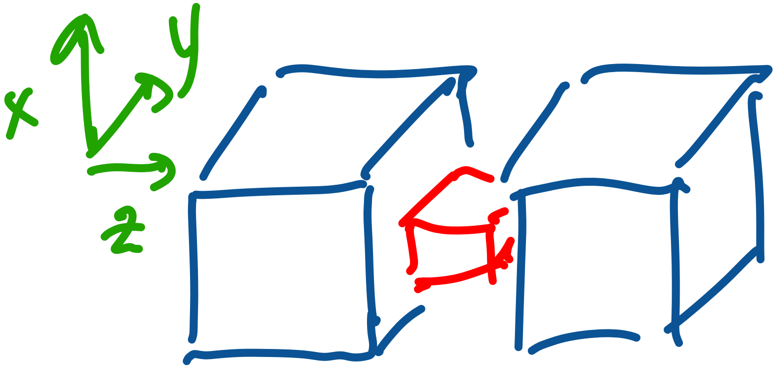
$N_{1D}(E)$?

BOUNDING BOX MODEL

FOR SOME CONDITION OF THE MOLECULAR SYSTEM IT COULD BE USED

HOW DOES CONDUCTION HAPPEN IN THIS SYSTEM?





0D SYSTEMS
QUANTUM DOT

ex. 3nm x 3nm x 3nm
(x) (y) (z)

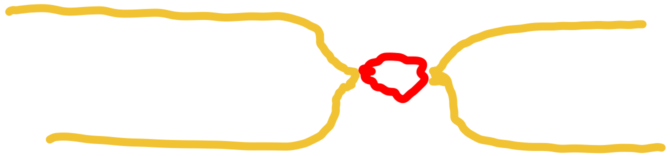
THE BOUNDING BOX APPROXIMATION DOES NOT GIVE A GOOD APPROXIMATION OF THE ALLOWED ENERGIES IN THE DOT

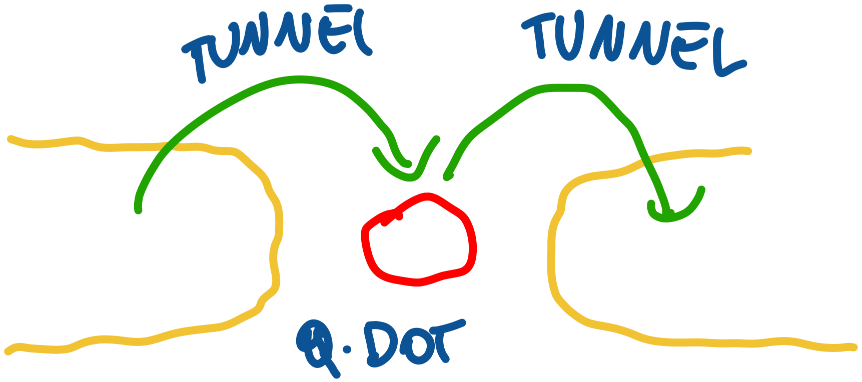
CONDUCTION DEPENDS ON COUPLING BW. DOT AND ELECTRODES

WEAK COUPLING → S.E.T.

STRONG COUPLING → MOLECULES

HOW DOES CONDUCTION HAPPEN IN THIS SYSTEM?

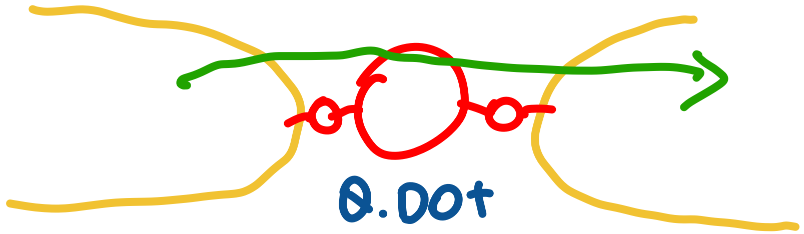




WEAK COUPLING

CURRENT IS THE RESULT OF A SEQUENTIAL TUNNELING PROCESS

S.E.T.



STRONG COUPLING

CHEMICAL BONDS

BONDS ALLOW THE FLOW OF ELECTRONS SIMILAR TO QUANTUM WIRE

MOLECULAR TRANSISTORS

MODEL FOR CONDUCTION IN STRONGLY COUPLED QUANTUM DOTS

→ COHERENT TRANSPORT OF ELECTRONS

FROM SOURCE ELECTRODE ↓

TO MOLECULE ↓

TO DRAIN ELECTRODE

THE FLOW DEPENDS ON

- N
- D.O.S.
- F

CONDUCTION IN S.C. QDOTS

→ N : NUMBER OF ELECTRONS

→ D.O.S: DENSITY OF STATES

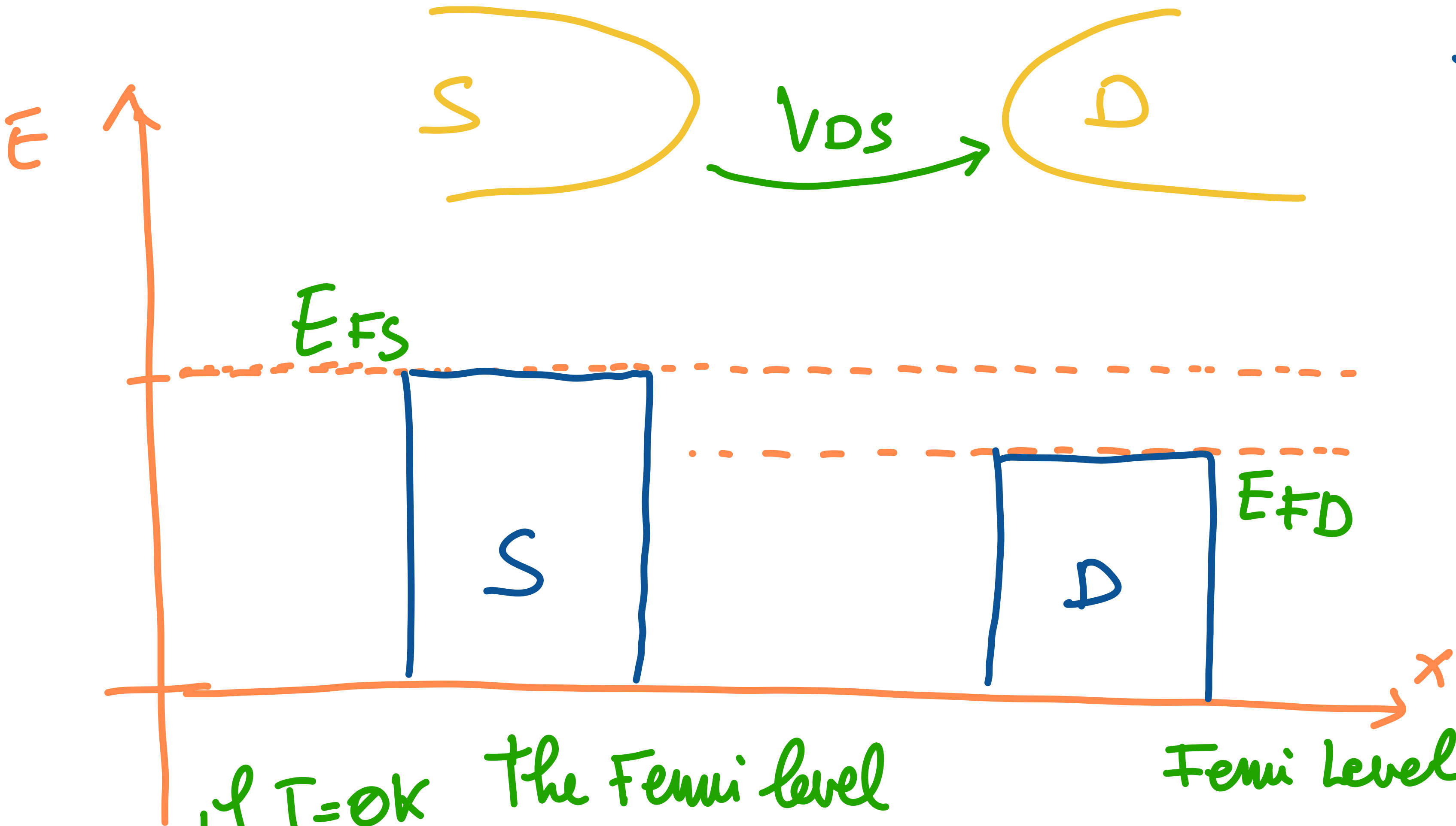
N. OF FREE STATES THAT AN ELECTRON CAN OCCUPY

(N. OF STATES IN A CONDUCTOR PER UNIT ENERGY)

→ F. : FERMI FUNCTION

PROBABILITY THAT THE STATE CAN BE OCCUPIED BY ELECTRON

CONDUCTION IN S.C. QDOTS



ELECTRODES ARE CHARGES RESERVOIRS

if T=0K the Fermi level E_{FS} FERMI LEVEL OF SORURCE

$> E_{FS}$ ALL STATES EMPTY

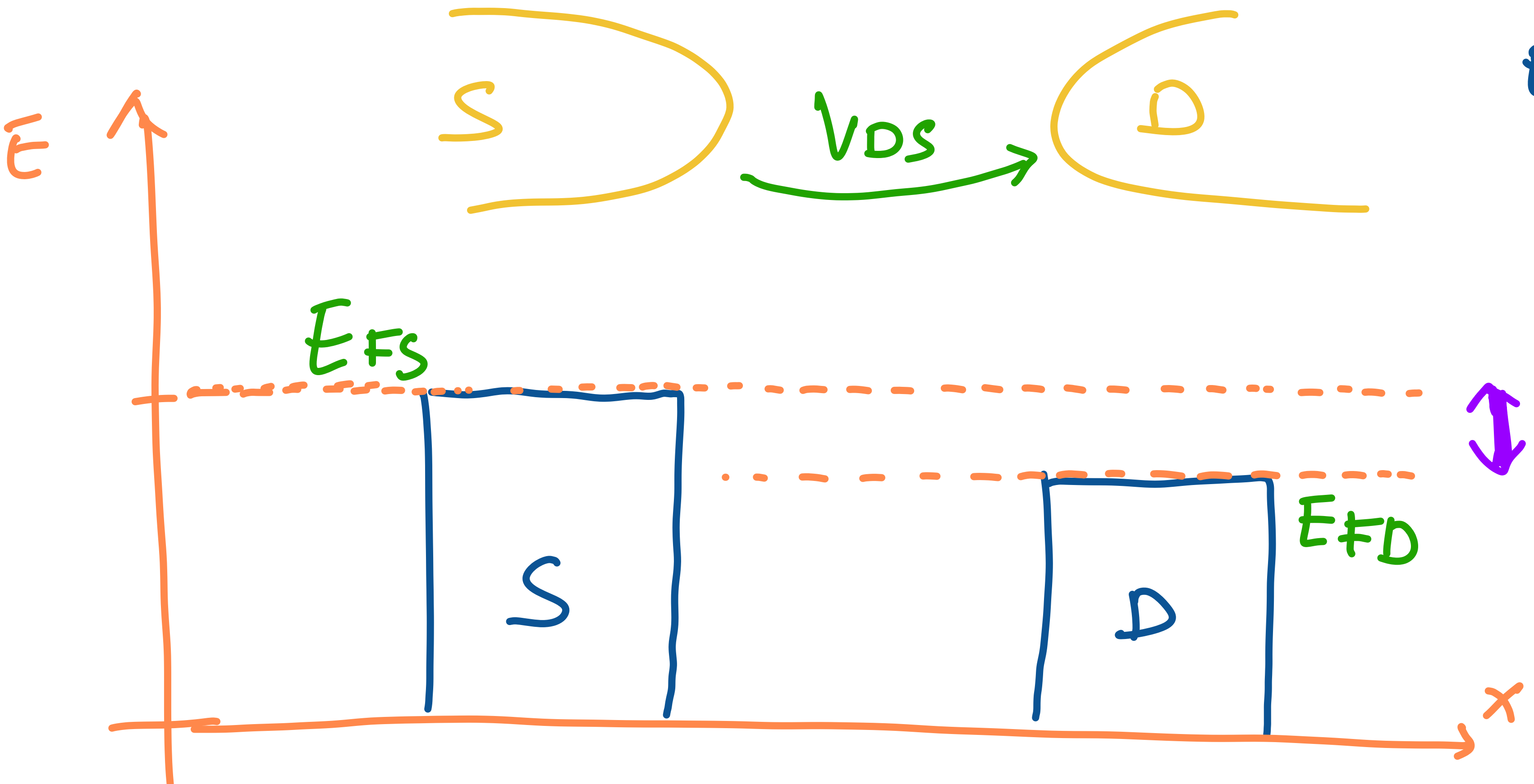
$< E_{FS}$ ALL STATES OCCUPIED

Fermi Level @ DRAIN E_{FD}

$> E_{FD}$ all states empty

$< E_{FD}$ all states occupied

CONDUCTION IN S.C. QDOTS



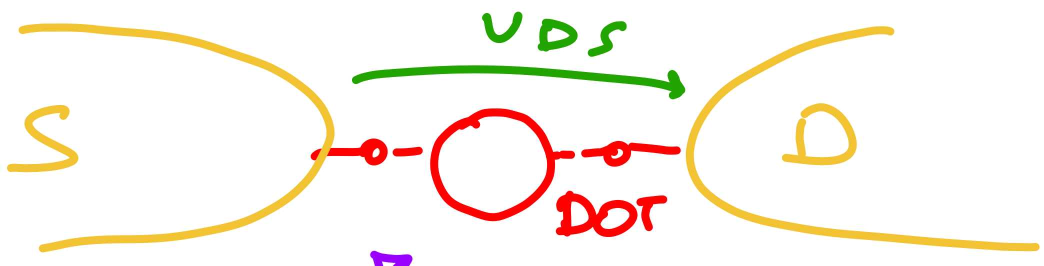
ELECTRODES ARE CHARGES RESERVOIRS

BIAS WINDOW

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

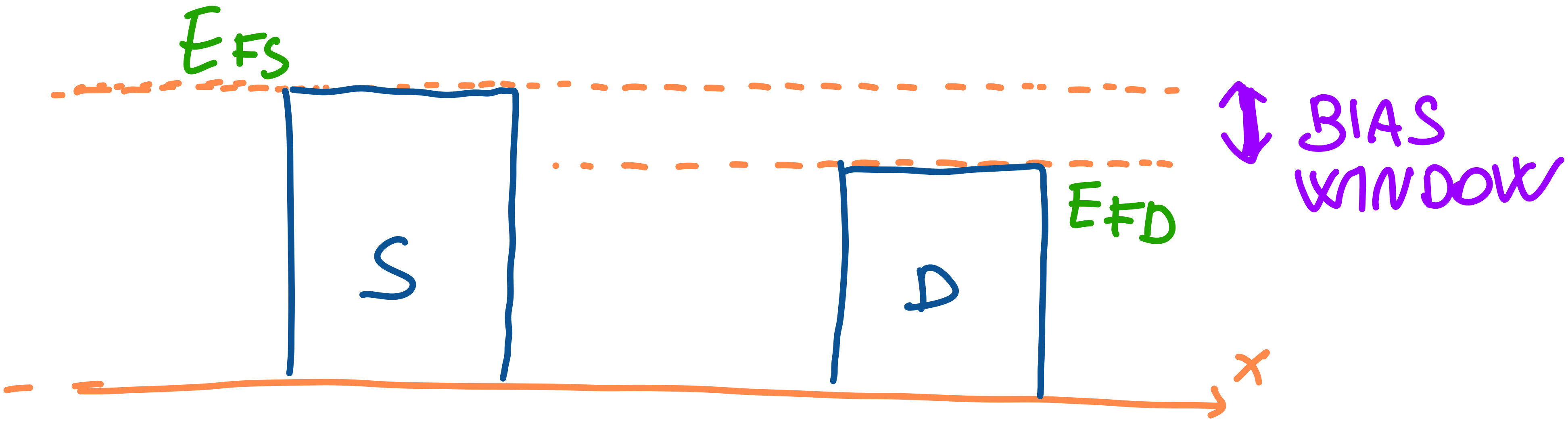
$$f(E, E_{FS}) = \frac{1}{1 + e^{\frac{E - E_{FS}}{kT}}} \qquad f(E, E_{FD}) = \frac{1}{1 + e^{\frac{E - E_{FD}}{kT}}}$$

CONDUCTION IN S.C. QDOTS



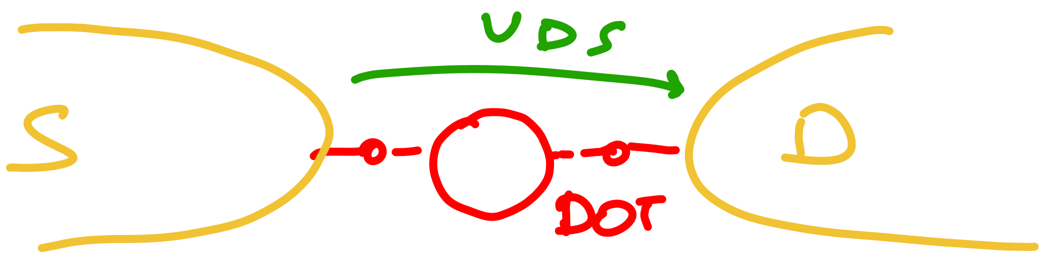
THE DOT CONTRIBUTES WITH N electrons e^- AT ENERGY E_L

THE DOT CONTRIBUTES WITH DISCRETE LEVELS OF POSSIBLE ENERGY STATES

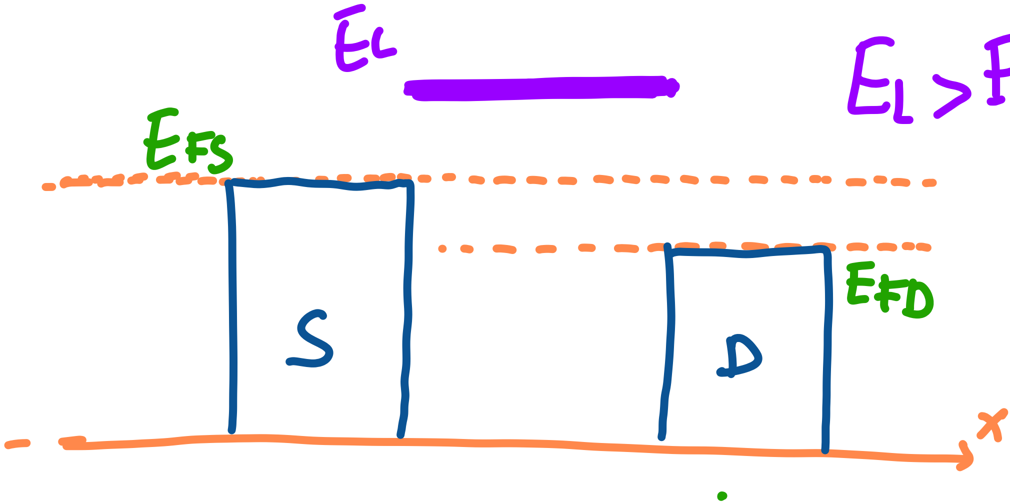


$\forall$ LEVEL $N : [0 \div 2]$

CONDUCTION IN S.C. QDOTS



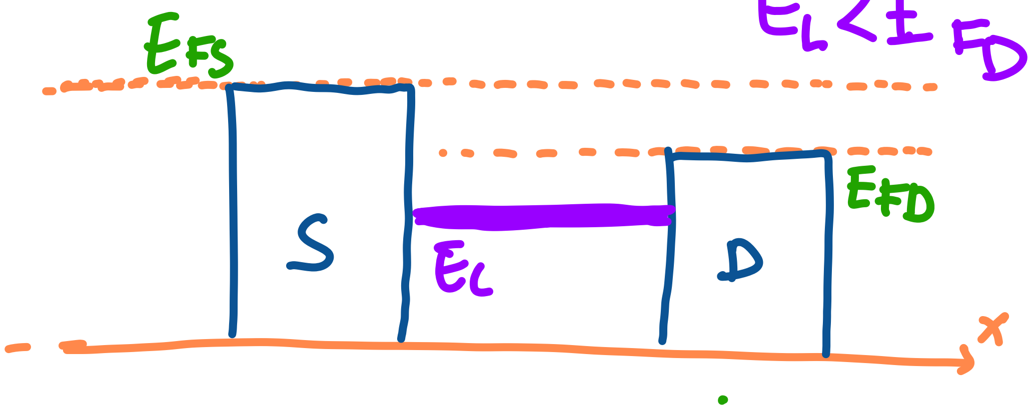
NO CONDUCTION



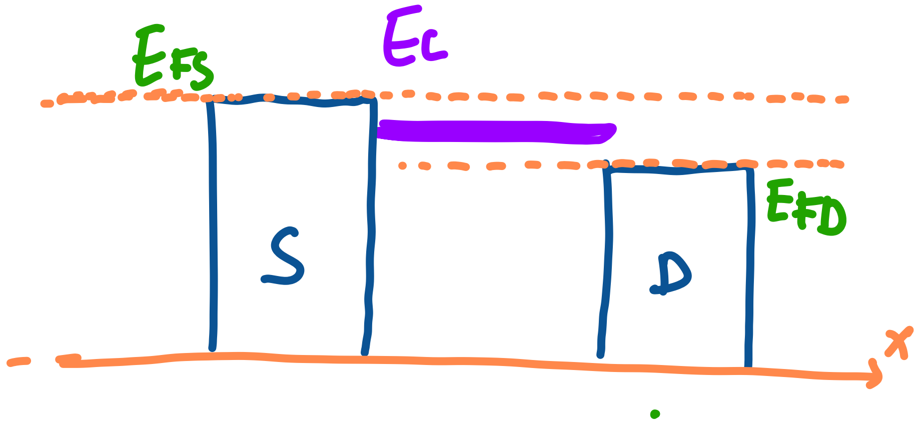
$E_L > E_{FS}$

NO CONDUCTION

$E_L < E_{FD}$

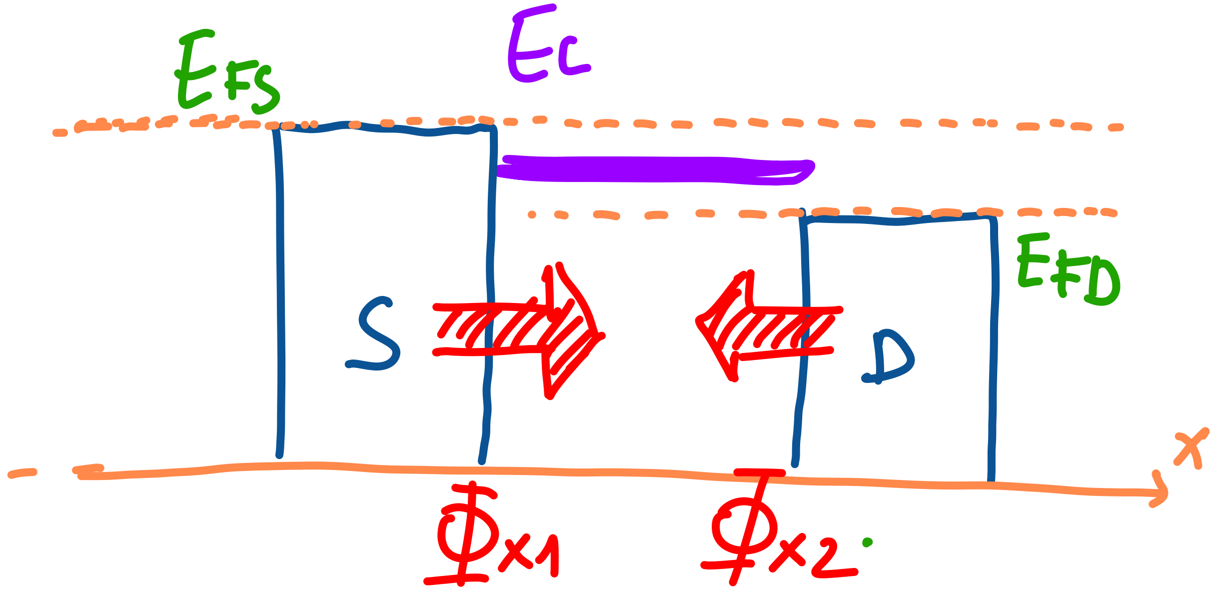


CONDUCTION



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

CONDUCTION IN S.C. QDOT



FLUXES OF ELECTRONS FROM ELECTRODES TO DOT

THE BOND B.W. DOT AND ELECTRODES QUALIFY THE INTERFACE AND THE TRANSFER TIME REQUIRED THE ELETRON TO MOVE FROM S TO DOT OR FROM S TO DOT

CONDUCTION IN S.C. QDOT

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

γ_1: COUPLING FACTOR B/W. SOURCE & DOT

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

γ_2: COUPLING FACTOR B/W DRAIN & DOT

CONDUCTION IN S.C. QDOT

$$\Phi_{X1 \to DOT} = \frac{2 \cdot f(E_L, E_{FS})}{\tau_1} = \frac{2\gamma_1 f(E_L, E_{FS})}{\hbar}$$

← FROM S TO DOT

$$\Phi_{DOT \to 1} = \frac{N}{\tau_1} = \frac{\gamma_1 \cdot N}{\hbar}$$

← FROM DOT TO S

$$\Phi_{X2 \to DOT} = \frac{2 f(E_L, E_{FD})}{\tau_2} = \frac{2\gamma_2 f(E_L, E_{FS})}{\hbar}$$

← FROM D. TO DOT

$$\Phi_{DOT \to 2} = \frac{N}{\tau_2} = \frac{\gamma_2 \cdot N}{\hbar}$$

← FROM DOT TO D.

CONDUCTION IN S.C. QDOT

NET FLUX $\Phi_{x1} = \frac{\gamma_1}{\hbar}\left[2f(E_L, E_{FS}) - N\right]$

NET FLUX $\Phi_{x2} = \frac{\gamma_2}{\hbar}\left[2f(E_L, E_{FS}) - N\right]$

DIFFERENCE BW. FLUX GOING IN AND OUT FROM ON ELECTRODE TO THE DOT

CONDUCTION W Q. DOT S. C.

FOR CONSERVATION OF CHARGE IN STEADY STATE

$$\Phi_{X_1} = -\Phi_{X_2}$$

SUBSTITUTIG → OBTAIN $\mathcal{N}$

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

see exercises to compute $\mathcal{N}$

CURRENT IN S.C. QD.

$$I_{DS} = q \cdot \Phi_{x1} \text{ netflux}$$

SUBSTITUTE Φ_{x1} and N

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

see exercises for examples

CONDUCTION IN MOLECULAR Q.D.

→ LEVEL BROADENING

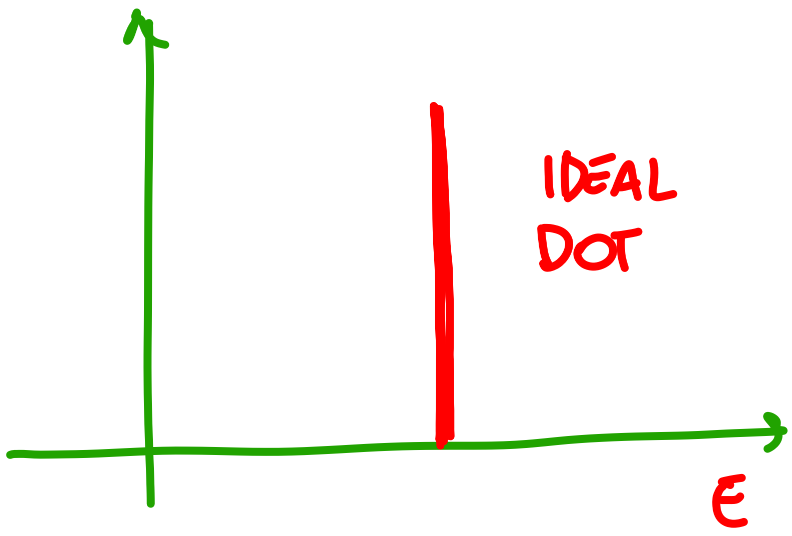
→ CHARGE EFFECT

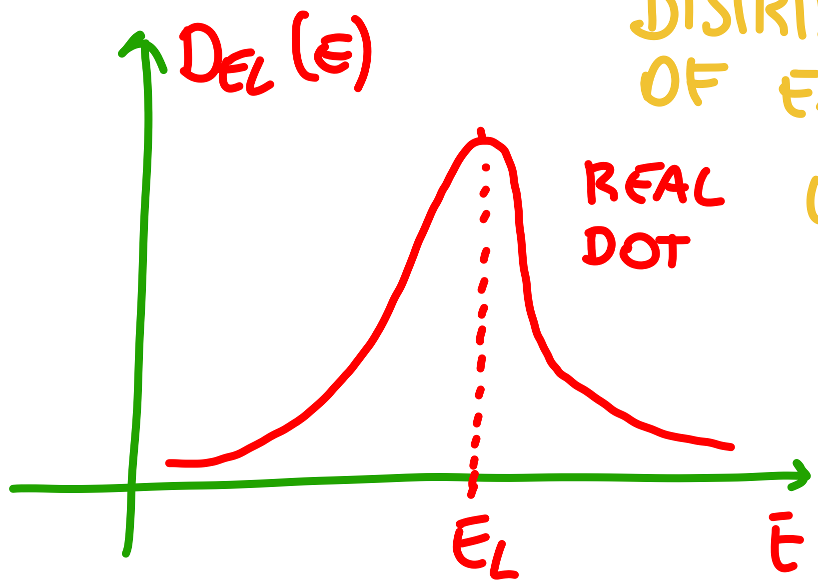
→ EXTERNAL SOURCES

CONDUCTION IN MOLECULAR Q.D

IN A <u>REAL DOT</u> e.g. MOLECULE

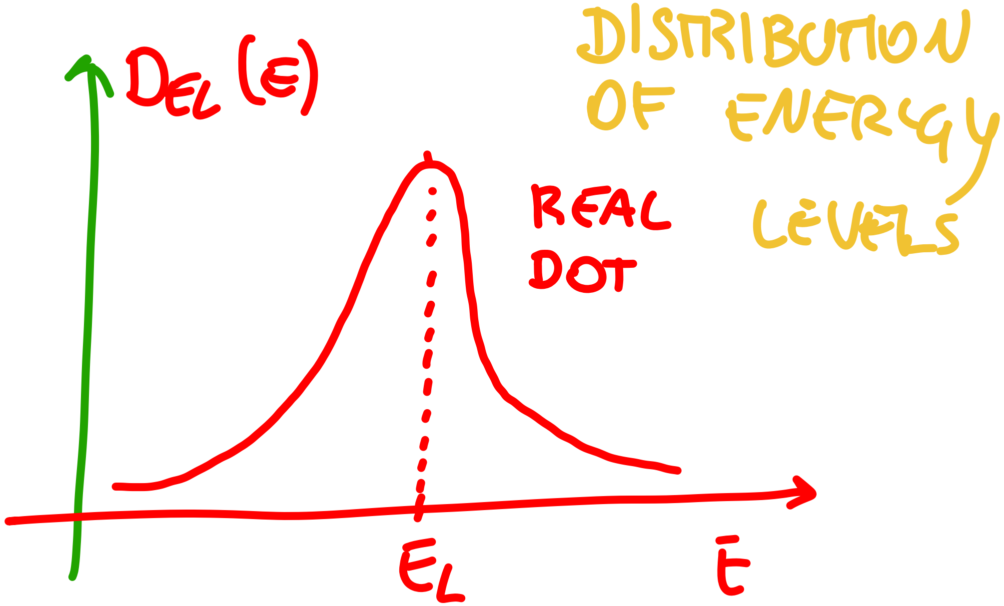
THE ENERGY LEVEL E_L IS NOT DISCRETE





DISTRIBUTION OF ENERGY LEVELS

LEVEL BROADENING



LORENZIAN DISTRIBUTION

$$D_{EL}(E) = \frac{\gamma/2\pi}{(E-E_L)^2 + \left(\frac{\gamma}{2}\right)^2}$$

CURRENT WITH BROADENING

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

.... SEE NEXT SLIDES

$$T(E) = 2\pi \frac{\gamma_1 \cdot \gamma_2}{\gamma_1 + \gamma_2} D_{EL}(E)$$

TRANSMISSION SPECTRUM

LANDAUER EQUATION

$$I_{DS} = \frac{2q}{h} \int T(E)\left[f(E, E_{FS}) - f(E, E_{FD}) \right] dE$$

↑

INCLUDES THE DOS OF COMPLEX MOLECULAR SYSTEMS

← DENSITY OF STATES

EPFL

MICRO-435 Quantum and Nanocomputing

Edoardo Charbon
Mariagrazia Graziano

MODELING OF MOLECULAR TRANSISTOR – PART 2

COMPLETE SIMPLE MODEL

THE TOTAL ENERGY

$$I_{DS} = \frac{q}{\hbar}\,\frac{2\gamma_1\gamma_2}{\gamma_1+\gamma_2}\int_{-\infty} D_{EL}(E-\mathbf{U})\cdot\left[f(E,E_{FS})-f(E,E_{FD})\right]dE$$

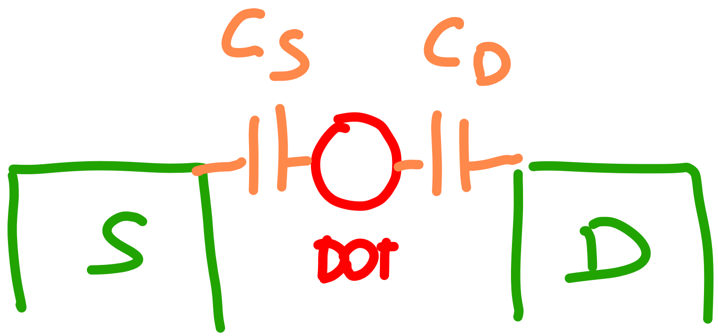
U? → GENERALIZATION FOR THE ENERGY OF THE SYSTEM USED TO MODEL OTHER EFFECTS ON THE SYSTEM

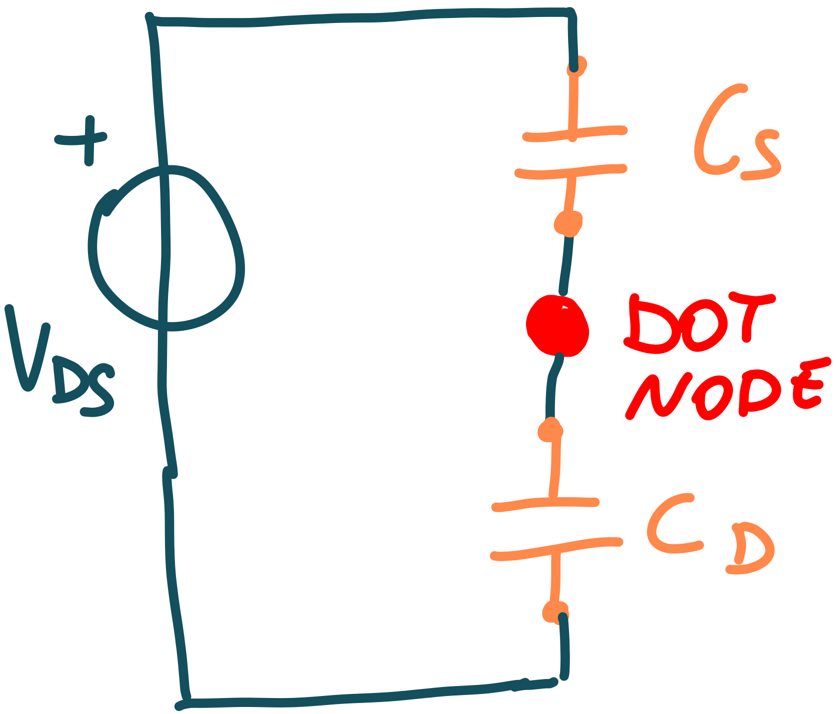
1) E_F OF DOT 2) CHARGE EFFECT 3) GATING

$$U = U_{V_{DS}} + U_{\substack{\text{CHARGING}\\\text{EFFECT}}} + U_{\text{GATING}}$$

(1) CONTRIBUTION OF V_{DS}

EQUIVALENT MODEL

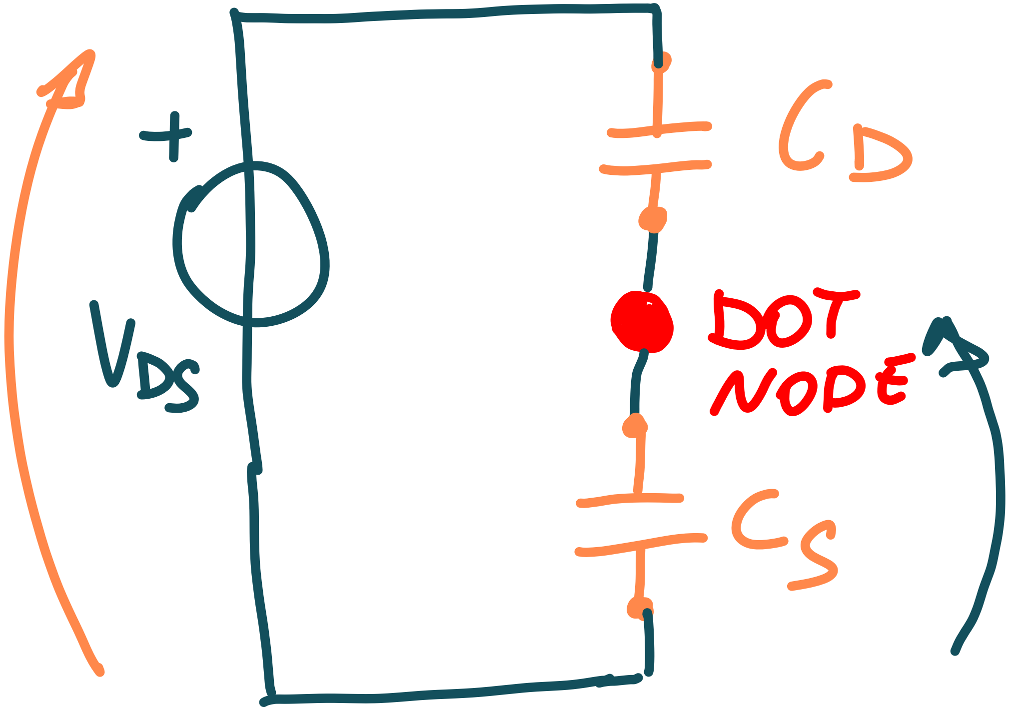




INTRUDUCE EQUIVALENT CAPACITANCES TO MODEL THE IMPACT ON ENERGY THROUGH THE 2 CONNECTIONS

CONTRIBUTION OF V_{DS}

CAPACITIVE DIVIDER



$V_{DOT}|_{V_{DS}}$

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

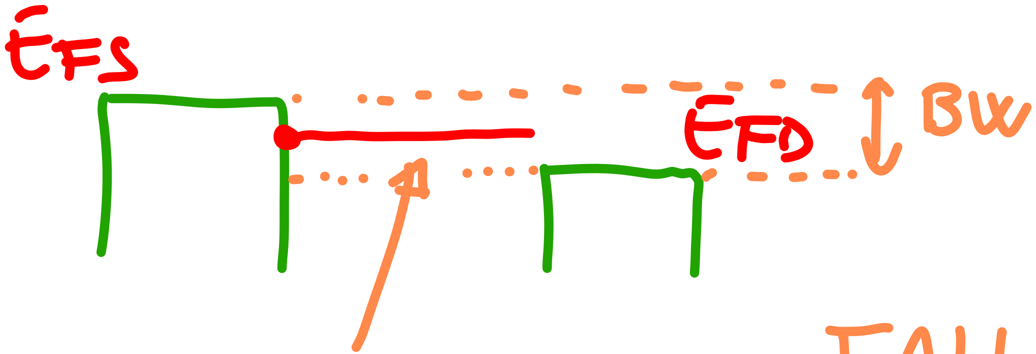
C_S and C_D RAPIRESENT THE QUALITY OF THE CONNECTION

CONTRIBUTION OF V_{DS}

- IF THE QUALITY OF THE 2 CONTACTS IS THE SAME $C_S = C_D \Rightarrow V_{dot} = \frac{1}{2} V_{DS}$

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

FOR THIS REASON



$E_L = E_{FDOT}$ FALLS IN THE MIDDLE OF BW IN THESE CONDITIONS

CONTRIBUTION OF V_{DS}

IN GENERAL

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

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

$T(E-U)$ CHANGES

IF DOT WELL CONNECTED TO SOURCE AND POORLY CONNECTED TO DRAIN $C_D \ll C_S$

$\Rightarrow E_{F\,DOT} \rightarrow$ NEAR E_{FS}

AND VICEVERSA

TYPICAL VALUES OF

$C_S \sim C_D$

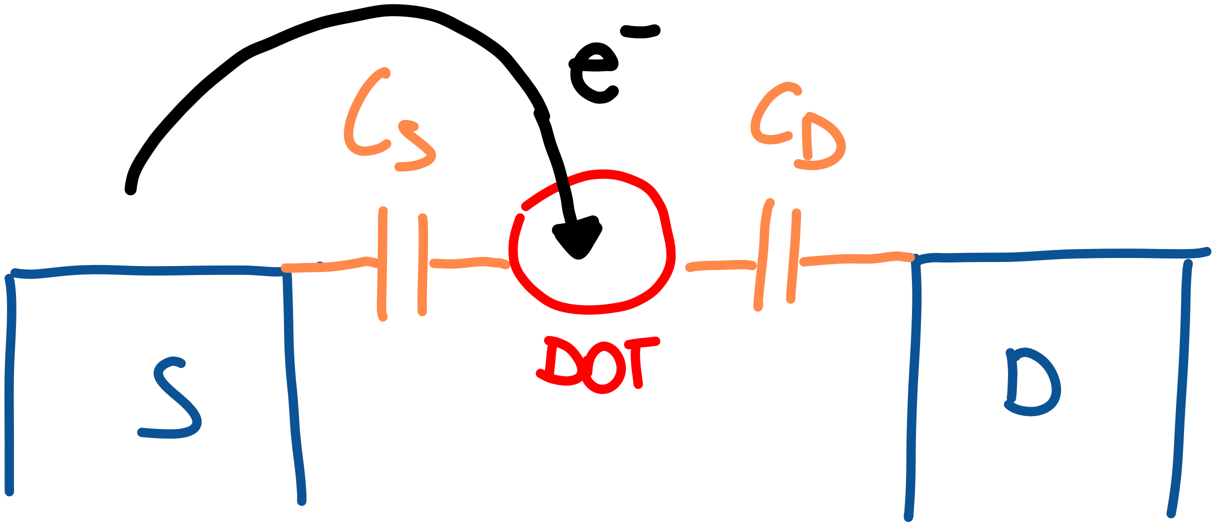
$\sim aF \sim 10^{-18}$

FEW attofarad

②

CHARGING EFFECT

NOT OBSERVED IN STANDARD SYSTEMS
(always present but has impact at nanoscale only)



STARTING MODEL

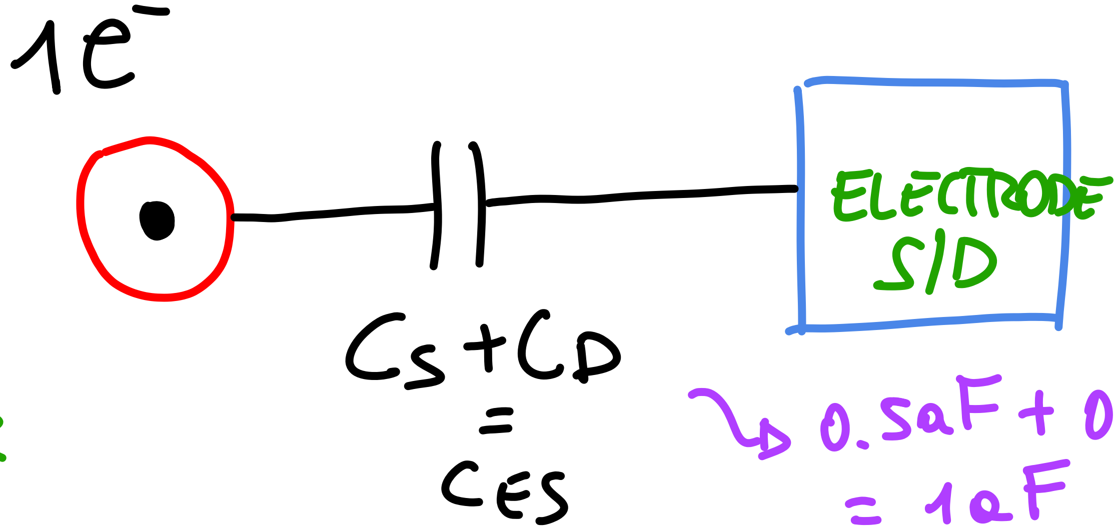
SOURCE AND DRAIN AT SAME POTENTIAL
$V_{DS}=0$

WHAT HAPPENS IF A CHARGE IS INJECTED IN THE DOT, WITH THE HYPOTHESIS OF NEUTRAL DOT

CHARGING EFFECT

REMODEL THE SYSTEM

- DOT IS A CHARGE CONTAINER
- S OR D IS ELECTRODE
- CAPACITANCE IS THE SUM (PARALLEL!)



$\to$ 0.5aF + 0.5aF = 1aF

ΔV VARIATION OF VOLTAGE

$\Downarrow$

ΔQ VARIATION OF CHARGE

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

(ΔQ $\leftarrow$ 1 electron)

CHARGING EFFECT

$$\Delta Q = -q \qquad C_{ES} = C_D + C_S$$

$$\Delta V = \frac{-q}{C_{ES}} = -\frac{1.6 \cdot 10^{-19}}{1 \cdot 10^{-18}} = -0.16\,V$$
$$= -160\,mV$$

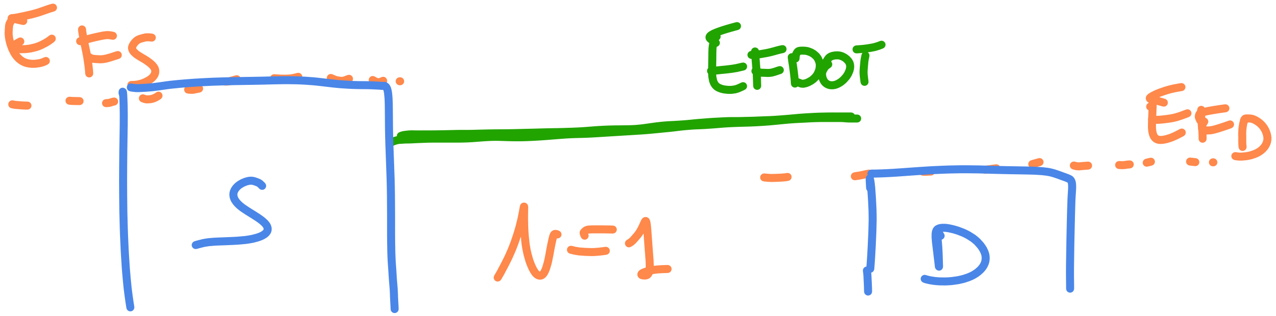
⇒ THE ELECTRON INJECTION SHIFTS THE VOLTAGE OF ~ 160 mV

$$U_{CHARGING-EFFECT} = -q\,\Delta V = \frac{q^2}{C_{ES}} \approx 0.16\,eV$$

⇒ SHIFT POTENTIAL ⇒ SHIFT D_{EL} ⇒ $T(E)$ ⇒ I_{DS}

CHARGING EFFECT $V_{DS} \neq 0$

NO CHARGING EFFECT



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

NEAR TO 1 (occupied states) — NEAR TO 0 (unoccupied states)

if $\gamma_1=\gamma_2$ $\boxed{N=1}$

If C.E. IS CONSIDERED

↓

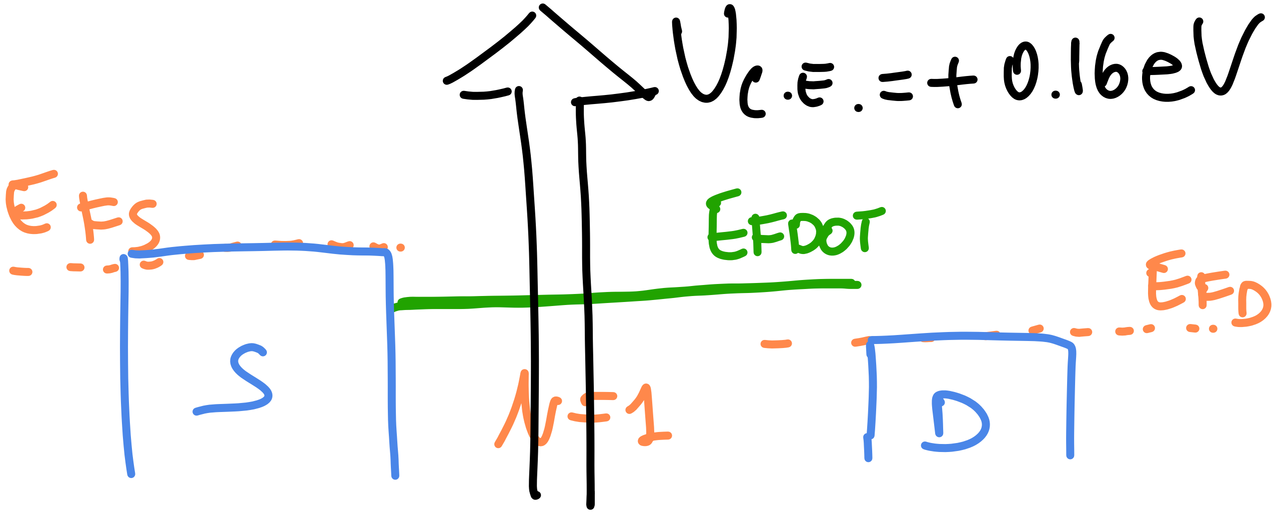
WHEN $1e^-$ JUMPS IN THE CHANNEL

↓

U CHANGES $\sim 0.16\,eV$

⇓

C.E.



THE $E_{LEVEL\,DOT}$ COULD ESCAPE FROM BW, THE CHARGE IN BW REDUCES !!!

???

SELF-CONSISTING FIELD : SCF

LET'S CONSIDER BROADENING ALSO

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

↑ DISTRIBUTION OF DENSITY OF STATES

↑ RESULT OF INTEGRATION

⇓

QUANTITY OF CHARGE

S.C.F.

$$U_{\text{CHARGING EFFECT}} = U_0 (N - N_0)$$

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

N_0 NUMBER OF ELECTRONS AT EQUILIBRIUM

N ACTUAL VALUE NUMBER OF ELECTRONS

SELF CONSISTING FIELD

$$N = \frac{2}{\gamma_1+\gamma_2}\int_{-\infty}^{+\infty} D_{EC}(E-U)\cdot\left[\;\cdots\cdots\;\right]dE$$

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

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

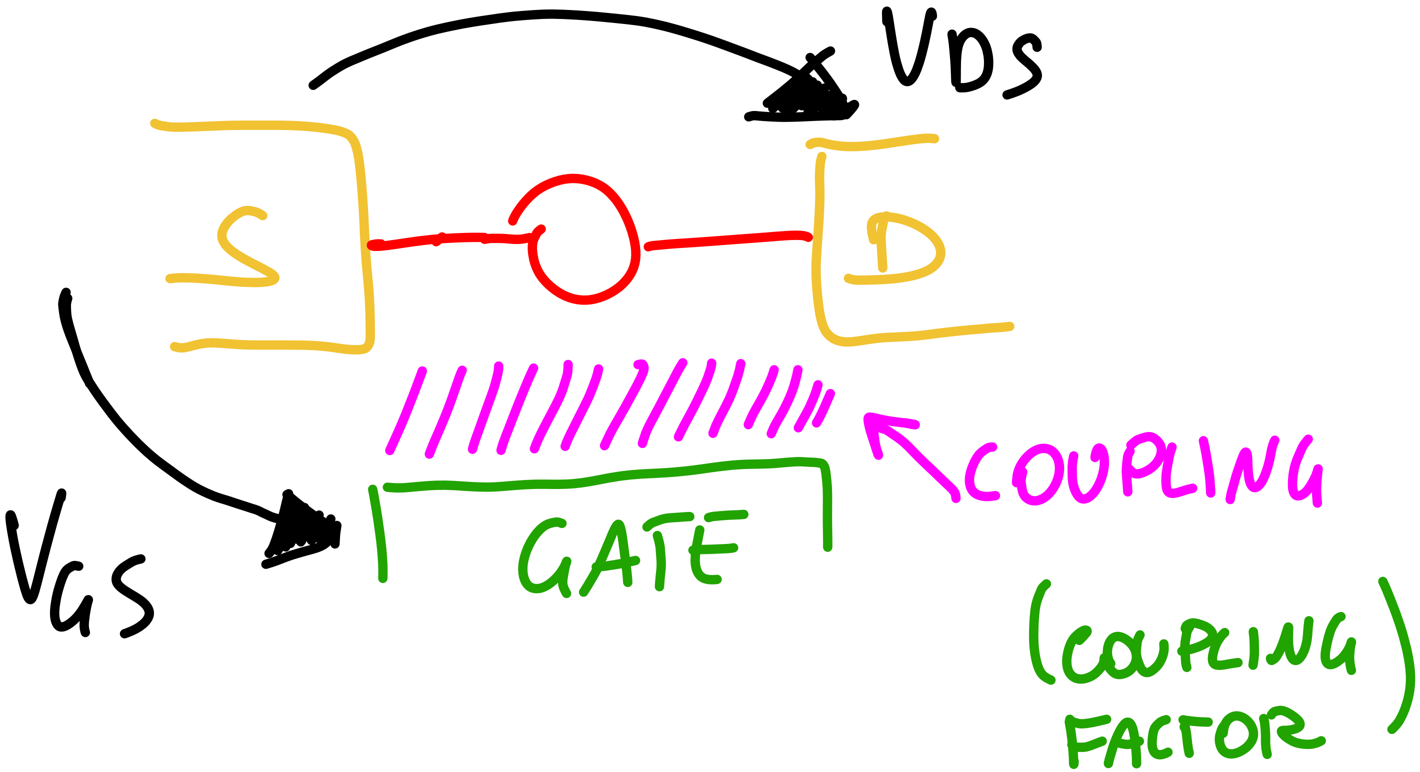
SCF LOOP

WHEN CONVERGENCY IS REACHED

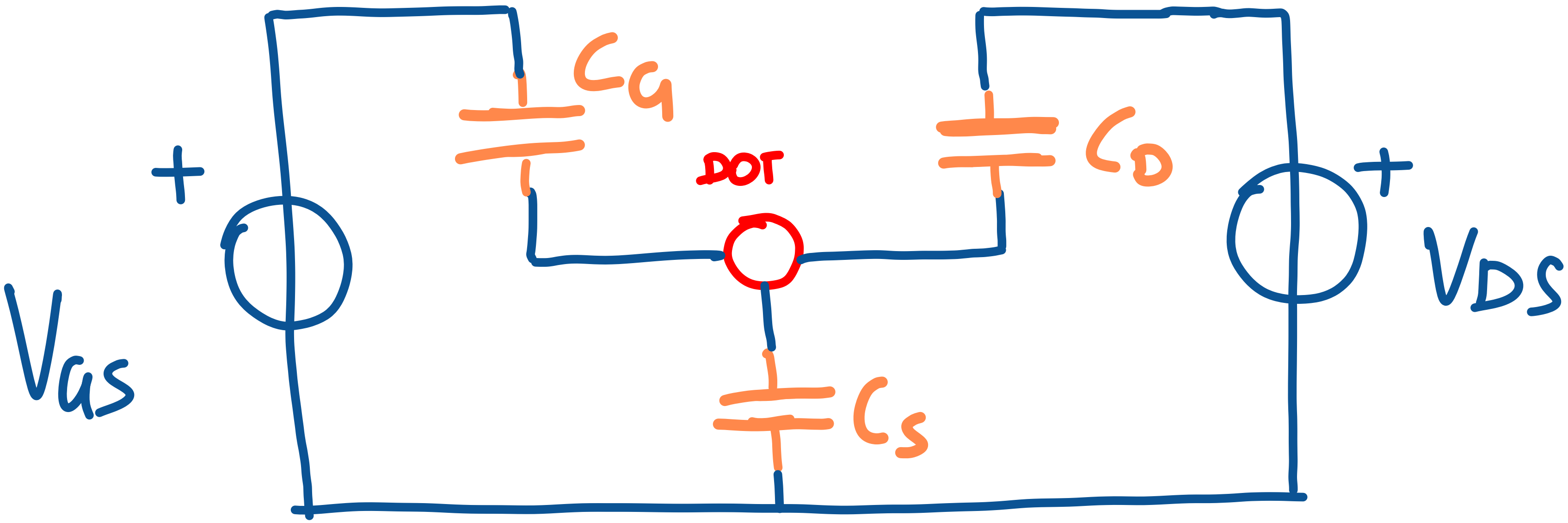
$$N \rightarrow U \rightarrow I_{DS}$$

③

GATING

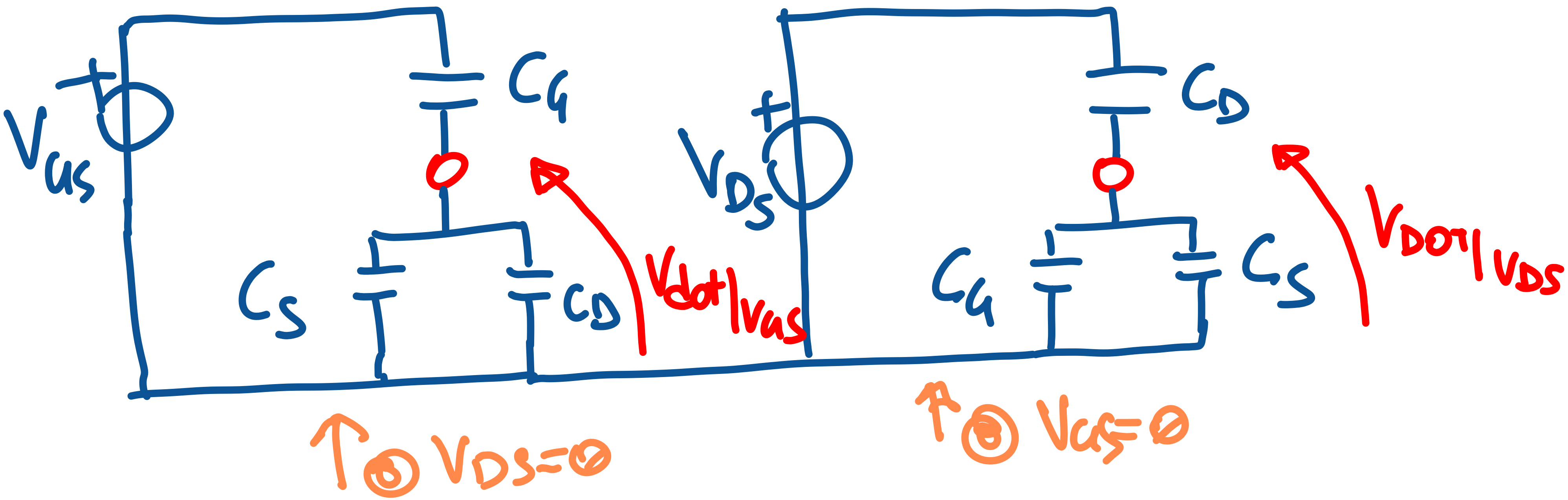


GATING IN CAPACITIVE MODEL



C_G MODELS THE CONTACT WITH THE GATE THROUGH A COUPLING FACTOR

SUPERPOSITION OF EFFECTS

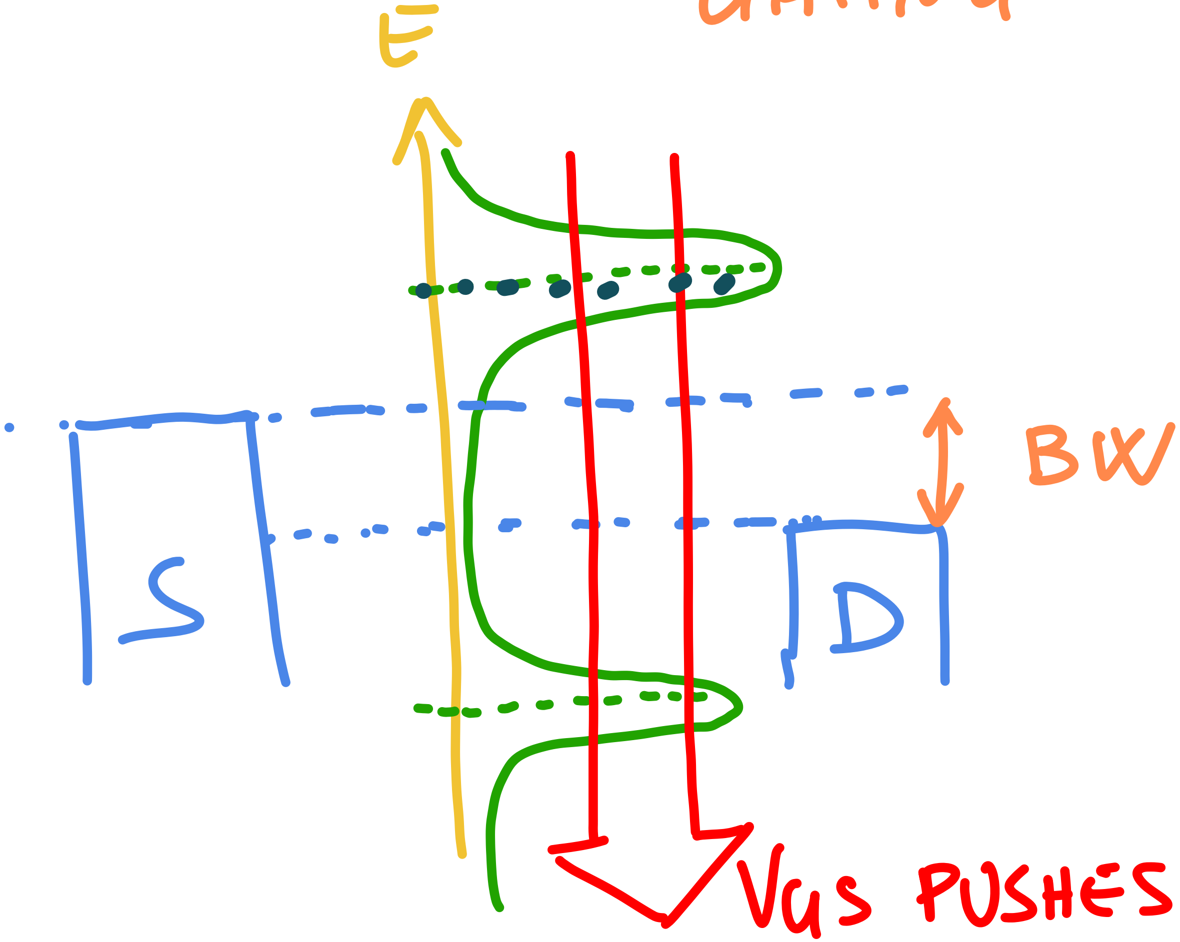


$$U_{V_{GS}} = -q\,V_{DOT}|_{V_{GS}} = -q\left(V_{GS}\cdot\frac{C_G}{C_G + C_S // C_D}\right) = -q\,V_{GS}\cdot\frac{C_G}{C_{ES}}$$

if $V_{GS} > 0$ $\quad U_{V_{GS}}$ ↓ TOWARD LOWER ENERGIES

if $V_{GS} < 0$ $\quad U_{V_{GS}}$ ↗ TOWARD HIGHER ENERGIES

GATING



example a case

WITH 2 E_L

WITH BROADENING

INITIALLY

NOT IN BW

V_{GS} PUSHES DOWN

↳ 1 PEAK MIGHT ENTER IN BW !!

$V_{GS} > 0$

$$U|_{V_{GS}} = -q \frac{C_G}{C_{ES}} V_{GS}$$

OVERALL

$$U = U_{V_{GS}} + U_{V_{DS}} + U_{CE}$$

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

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

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

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

↑ TO BE CONSIDERED WITH V_G