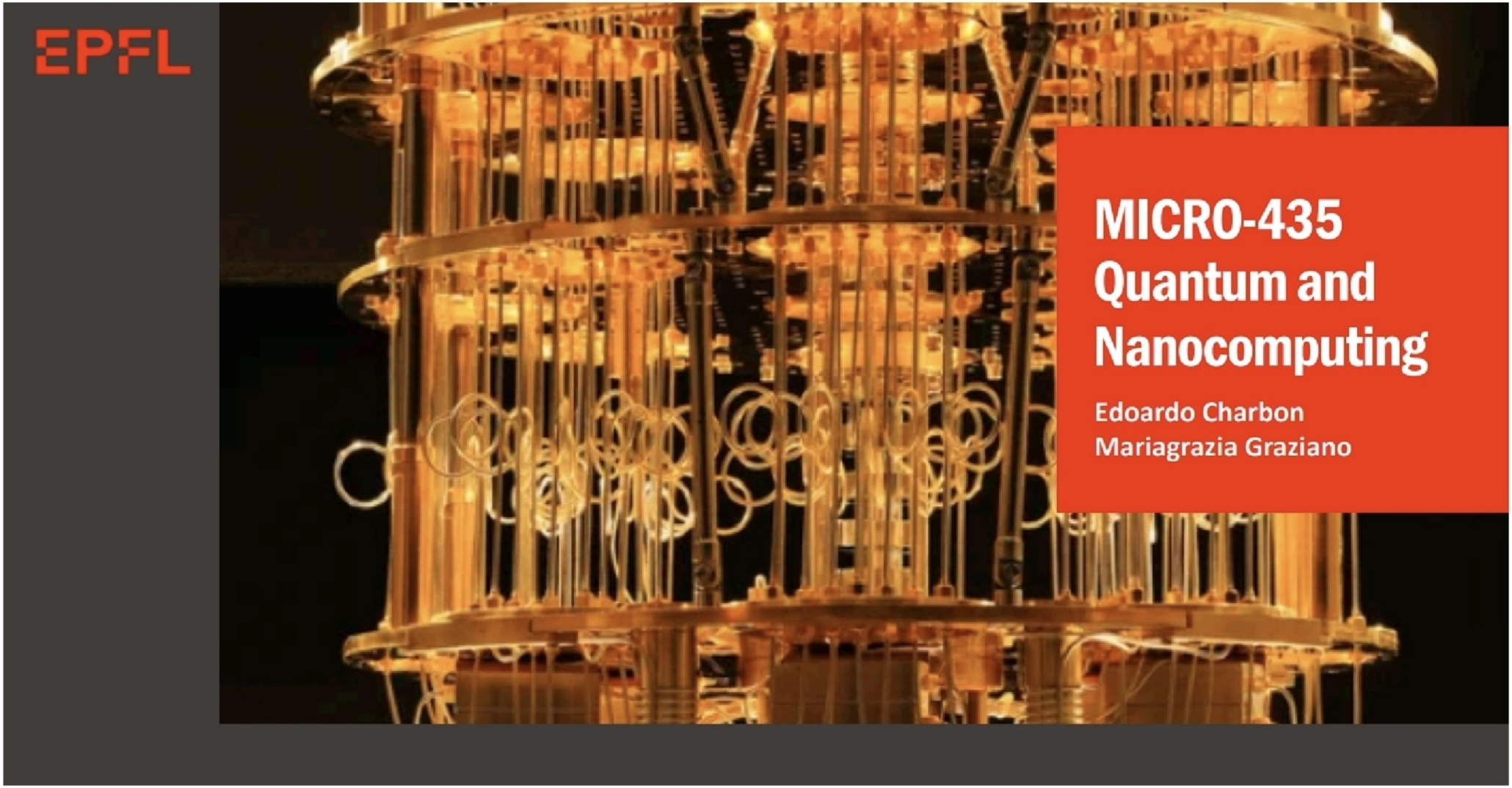


HT - EXERCISE

M. GRAZIANO - G. PICCININI

HT CONDUCTION EXERCISES

1

CONSIDERING THE MODEL BASED ON DISCRETE LEVELS, NO C. EFFECT, NO GATING

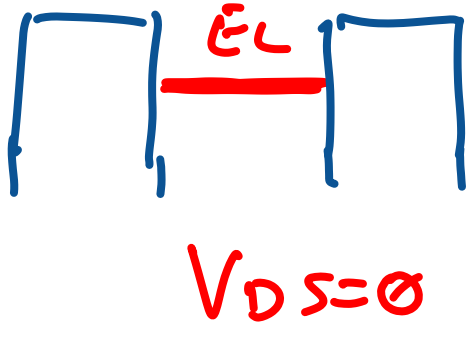
IN CASE OF 1 DISCRETE LEVEL IN THE DOT

CALCULATE N (APPROX) and I_{DS} (approx)

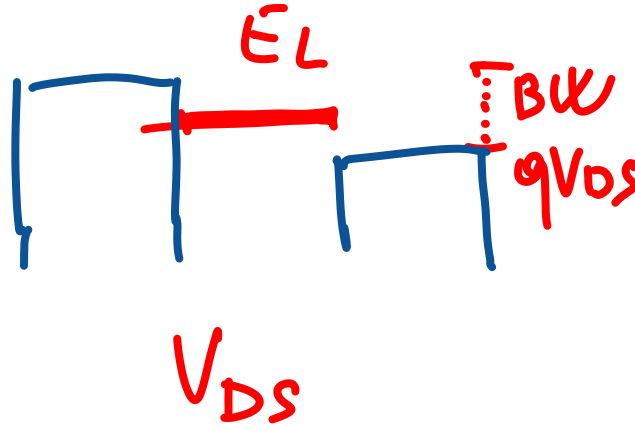
IN CASE a) b) c) WITH $\gamma_1 = \gamma_2$

a)

b)



c)



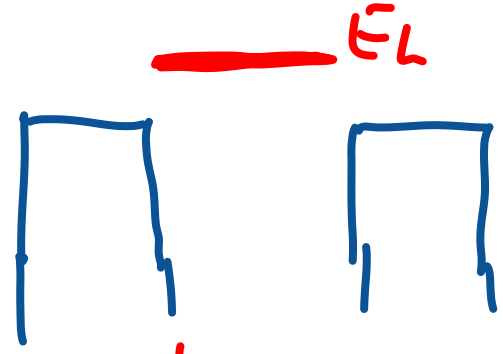
$$I_{DS} = \frac{q}{\hbar}\frac{2\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[f(E_L,E_{FS}) - f(E_L,E_{DS})\right]$$

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

FOR 1 DISCRETE LEVEL IN THE DOT

$\frac{\partial f}{\partial x}$

a)



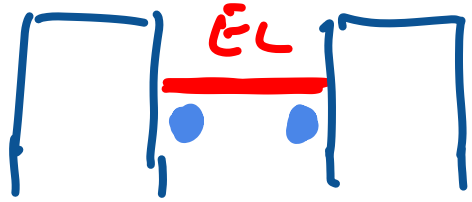
$V_{DS}=0$

$N=0$

$I_{DS}=0$

$f \rightarrow$ UNOCCUPIED $=0$

b)



$V_{DS}=0$

$f \rightarrow 1$ completely filled

$N \simeq 2$

$I_{DS}=0$

c)

V_{DS}

FILLED $f \rightarrow 1$

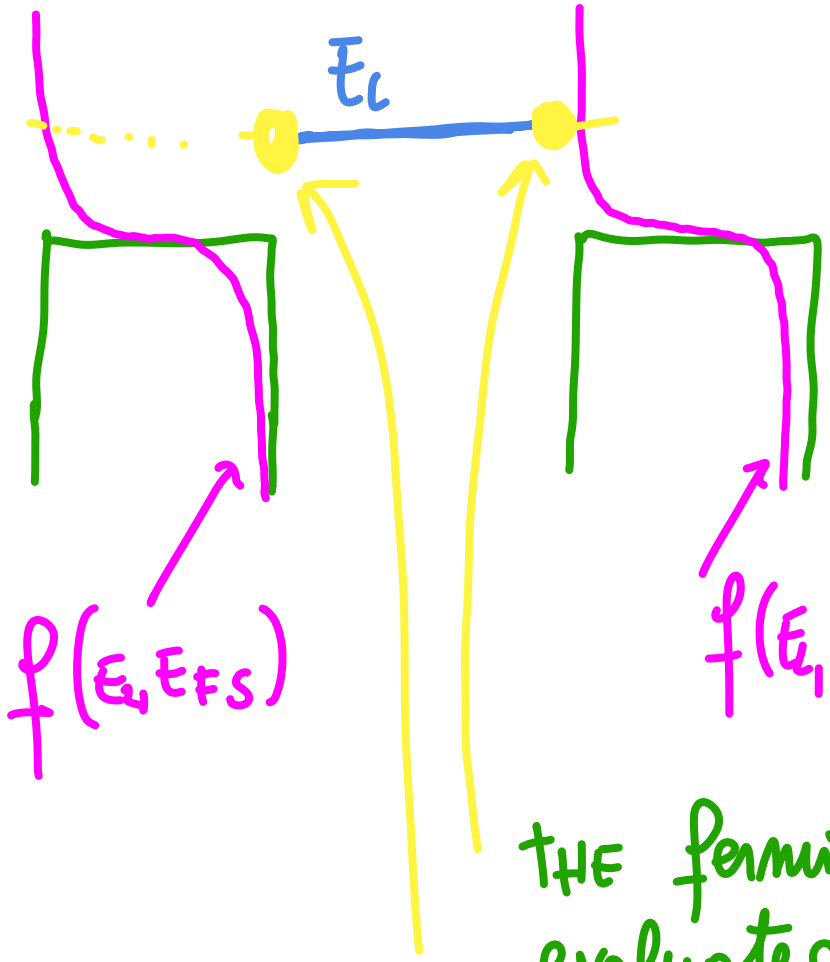
UNOCCUPIED $f \rightarrow 0$

$N \simeq 1$

$I_{DS} \simeq \frac{q}{\hbar}\gamma$

A COUPLE OF COMMENTS ON THE FERMI FUNCTIONS

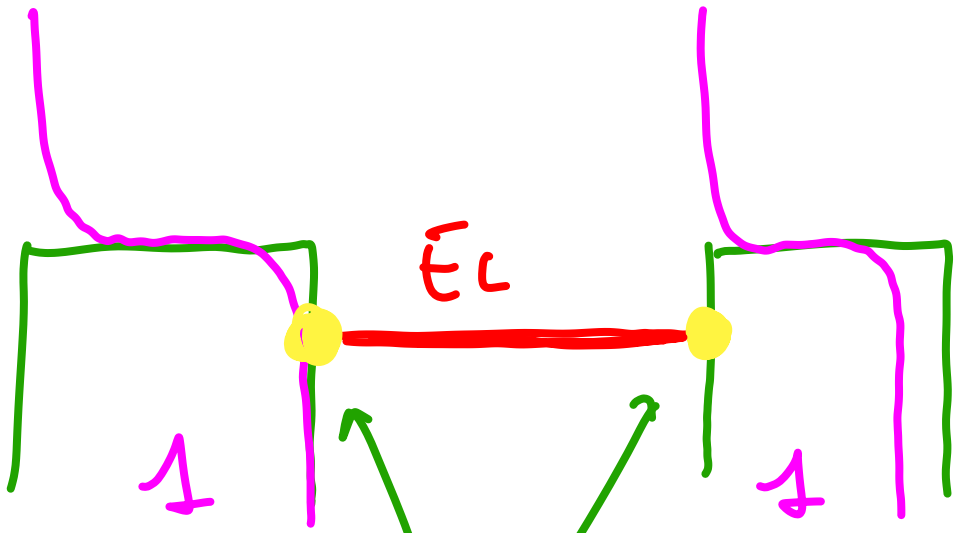
Q)



at $T \sim 300K$ the fermi functions are near to a step functions

THE fermi function of source and drain evaluated at the value E_L of the DOT are approximately $0 \rightarrow$ probability to find charge $= 0$

CASE b)



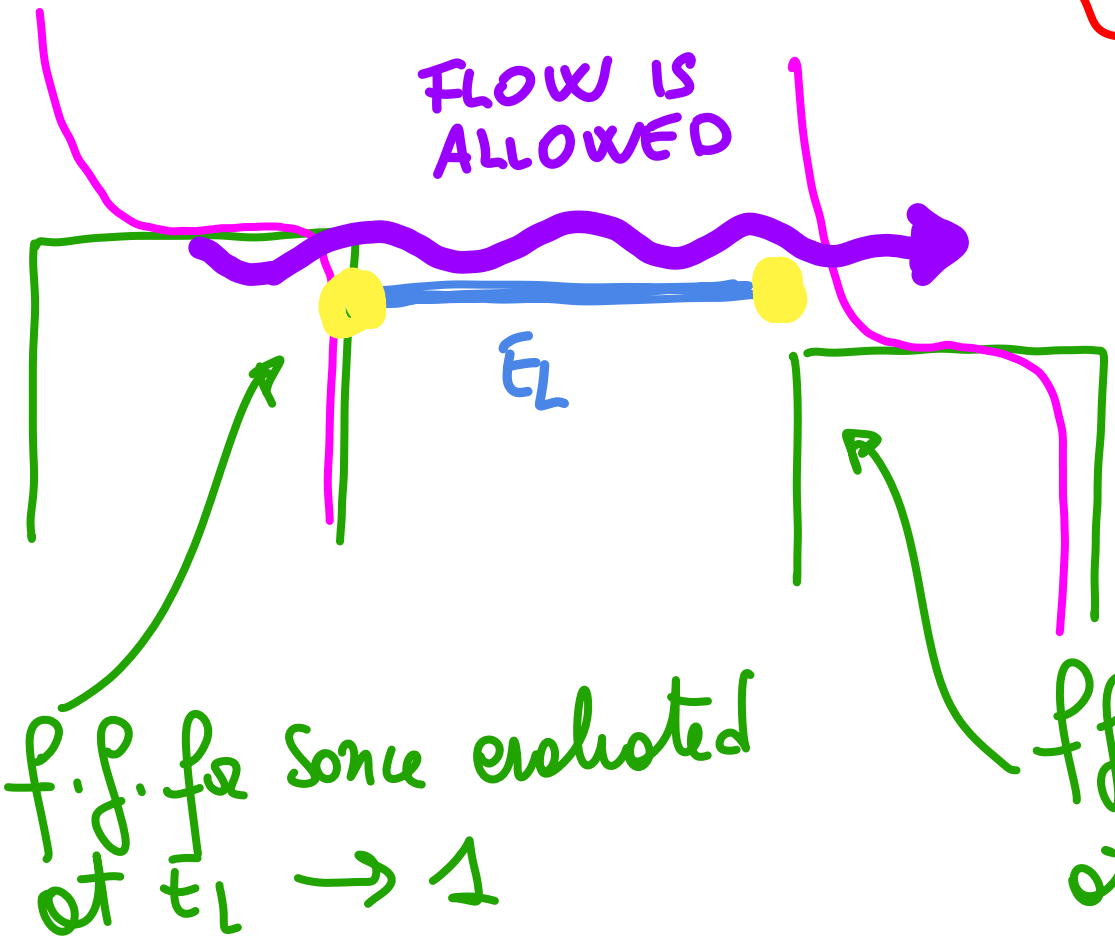
the f.f. of S. and d. evaluated at the level of the dot are approximately 1

→ probability to find a charge = 1

The no of electron is 2, but they do not find a flux, they cannot be hosted in the DRAIN

Case C)

- SOURCE IS PROVIDING A CHARGE (FILLED)



↳ DOT IS ALLOWING THE CHARGE TO MOVE

↳ DRAIN IS ACCEPTING AS IT IS NOT FILLED

f.f. for source evaluated at $t_L \rightarrow 1$

ff for drain evaluated at $E_L \rightarrow 0$

2

CONSIDERING THE MODEL BASED ON DISCRETE LEVELS, NO C. EFFECT, NO GATING

CALCULATE N and I_{DS}

IN TWO CASES OF MOLECULE

1.1) A LUMO TYPE MOLECULE WITH

$E_{L1} = 0.5eV$

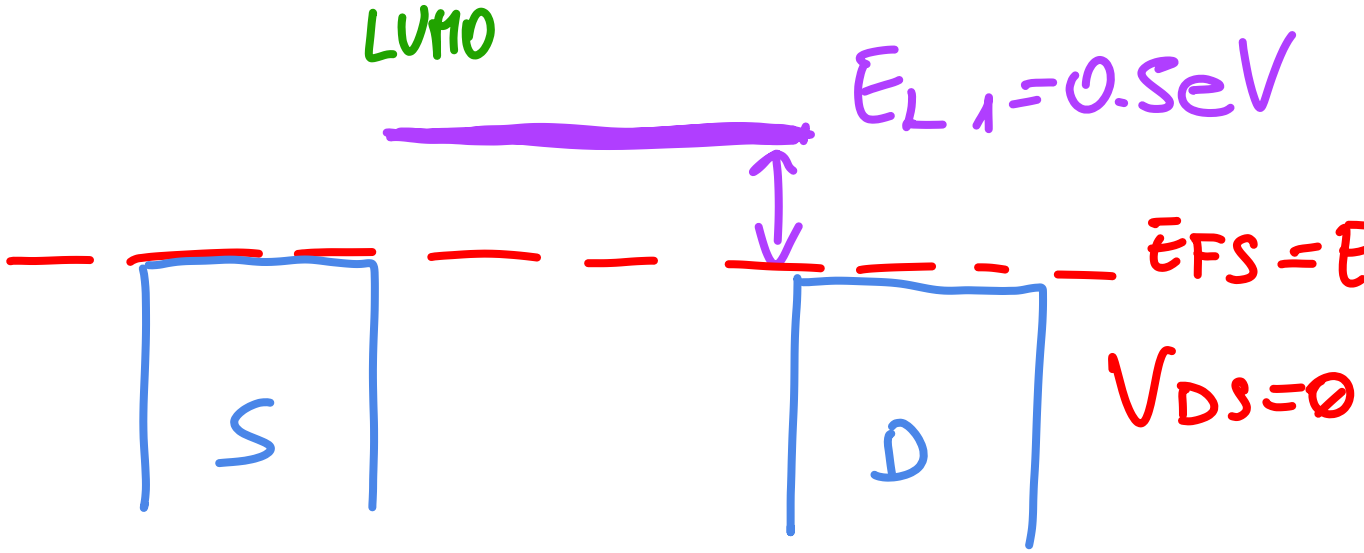
a) $V_{DS}=0V$ b) $V_{DS}=0.5V$ c) $V_{DS}=1V$

1.2) A HOMO TYPE MOLECULE WITH

$E_{L2} = 0.7eV$

a) $V_{DS}=0V$ b) $V_{DS}=0.7V$ c) $V_{DS}=1.4V$

1.1 $E_{L1} = 0.5eV$ a) $V_{DS} = 0V$



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

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

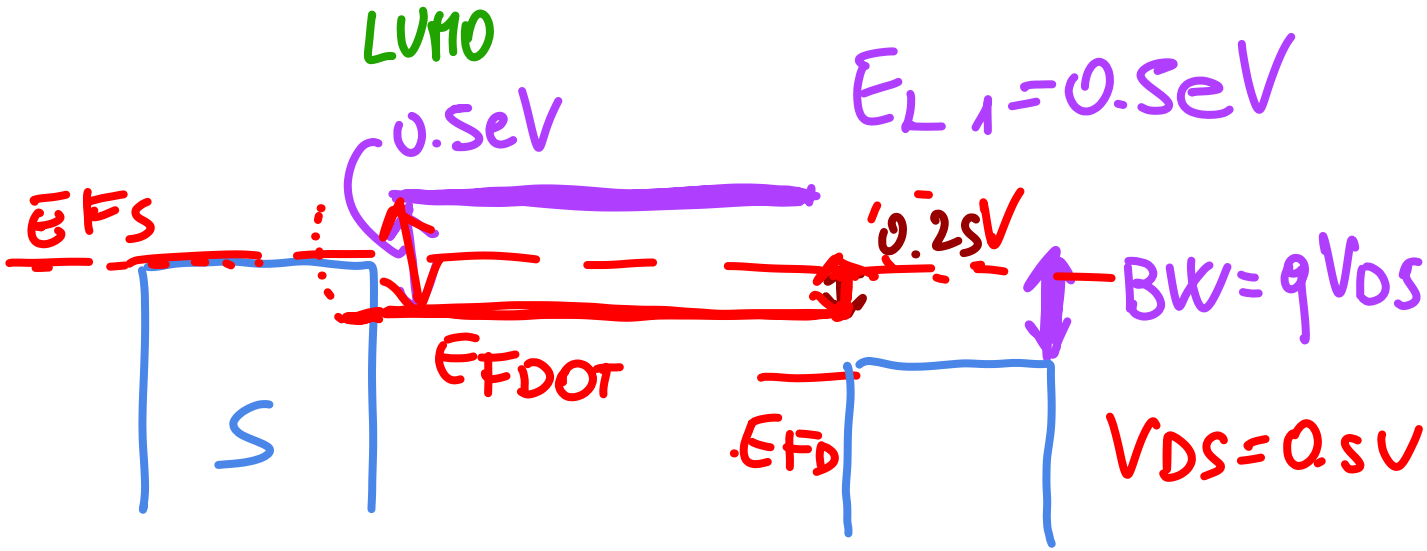
$f(E_L,E_{FS}) \to 0$

$f(E_L,E_{FD}) \to 0$

$N = 0$

$I_{DS} = 0$

1.1 $E_{L_1} = 0.5eV$ b) $V_{DS} = 0.5V$



$E_{FDOT} = \frac{1}{2} qV_{DS}$
$= 0.25V$

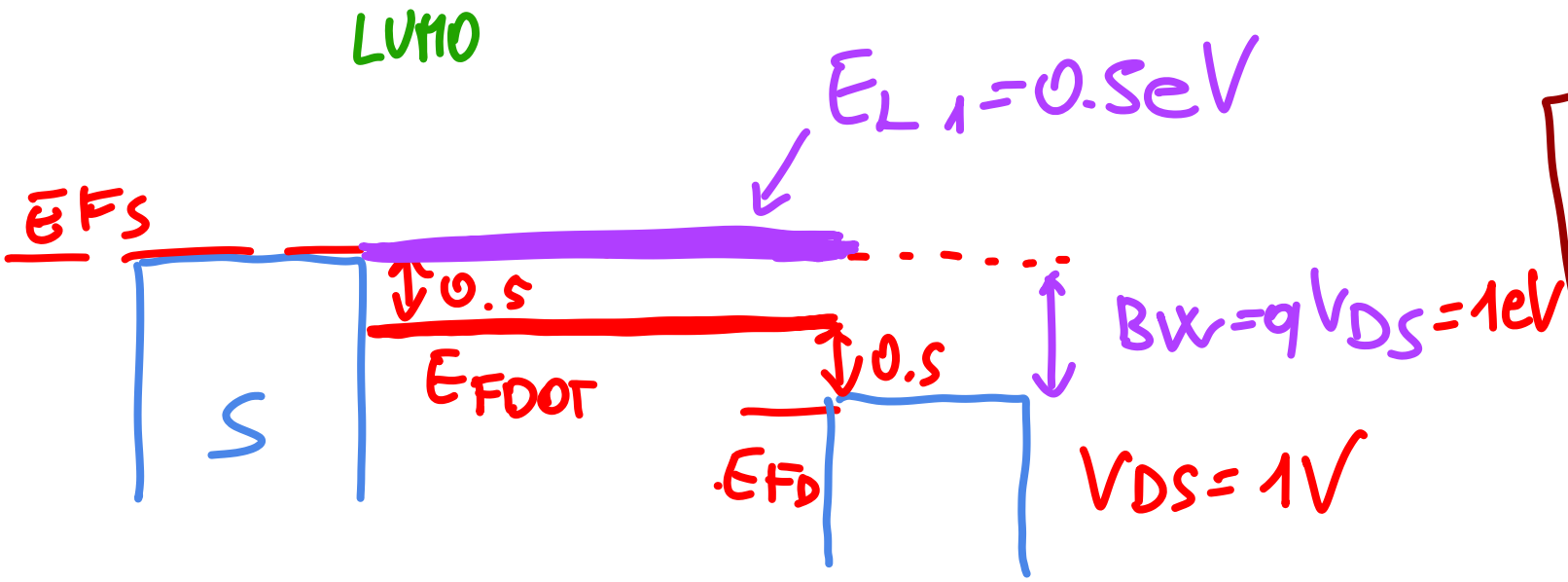
$f(E_L, E_{FS}) \to 0$
$f(E_L, E_{FD}) \to 0$

$N = 0$
$I_{DS} \approx 0$

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

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

1.1 $E_{L_1} = 0.5eV$ c) $V_{DS} = 1\,V$



$$E_{FDOT} = \frac{1}{2} q V_{DS} = 0.5\,V$$

$$f(E_L, E_{FS}) \to 1$$

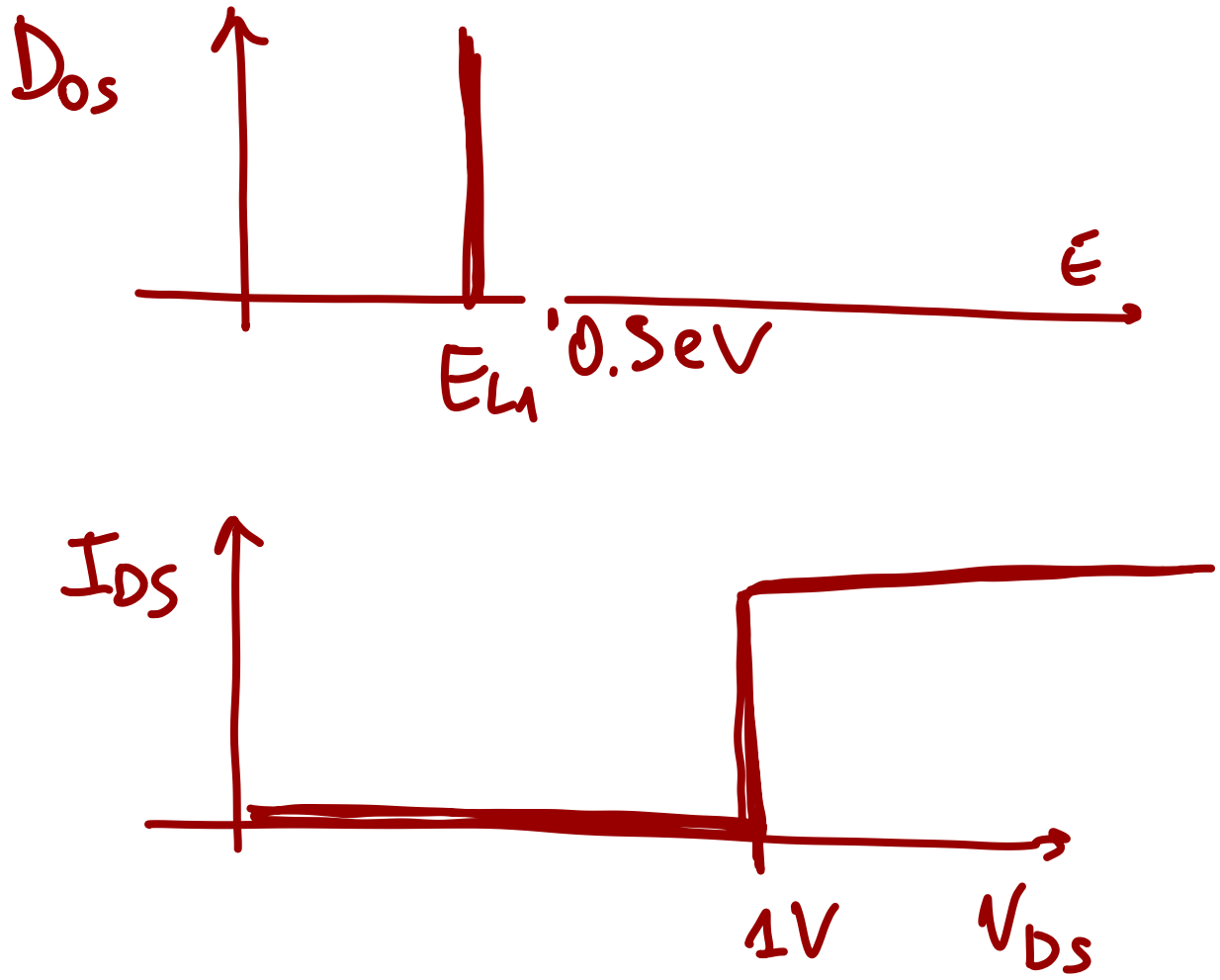
$$f(E_L, E_{FD}) \to 0$$

$$N = 1$$

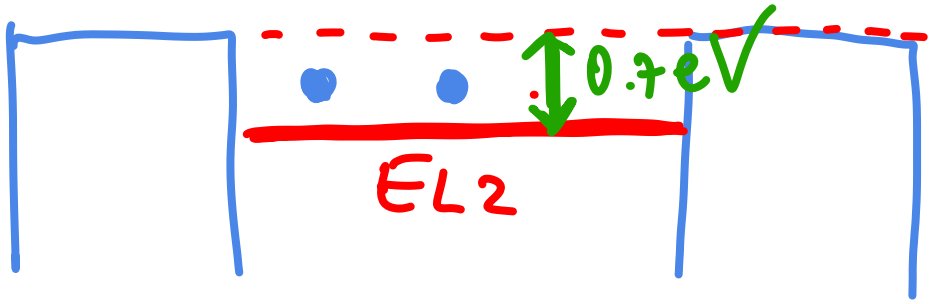
$$I_{DS} = \frac{q}{\hbar} \cdot \frac{2\gamma_1\gamma_2}{\gamma_1+\gamma_2}\left[f(E_L,E_{FS}) - f(E_L,E_{FD})\right]$$

$$I_{DS} \approx \frac{q}{\hbar} \cdot \frac{2\gamma_1\gamma_2}{\gamma_1+\gamma_2}$$

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

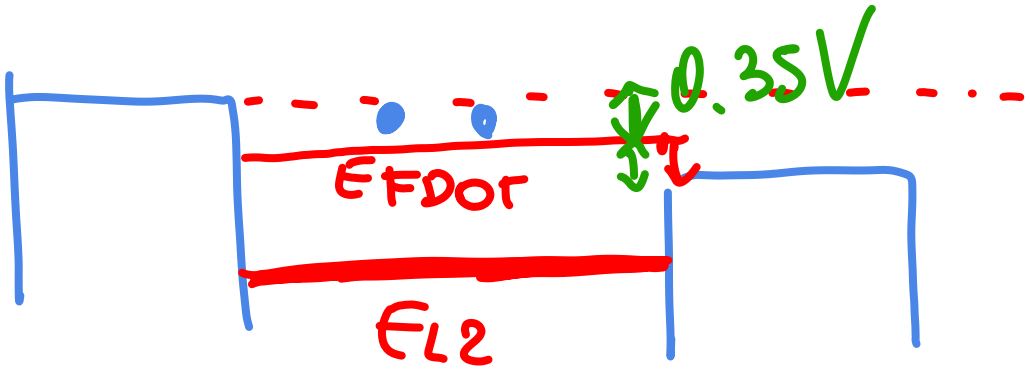

DOS
E
EL1 ~0.5eV
IDS
1V
VDS

1.2 HOMO $E_{L2} = 0.7eV$



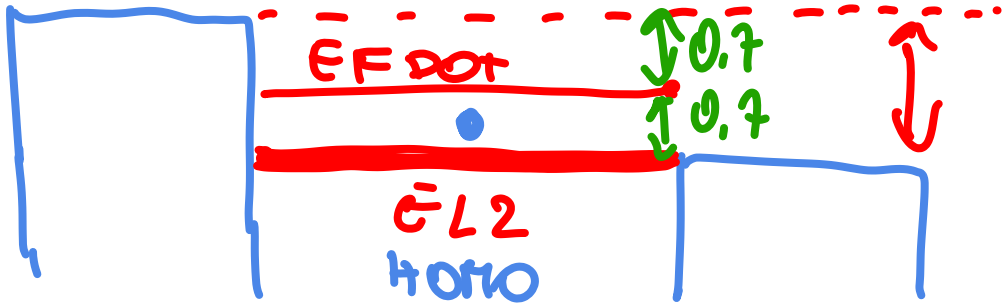
$V_{DS} = 0V$

$f_S \to 1$ $f_D \to 1$
$N = 2$
$I = 0$



$V_{DS} = 0.7V$

$f_S \to 1$
$f_D \to 1$
$N = 2$
$I = 0$

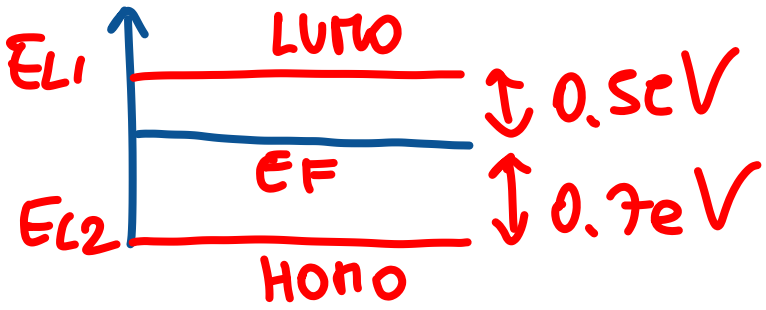


$V_{DS} = 1.4V$

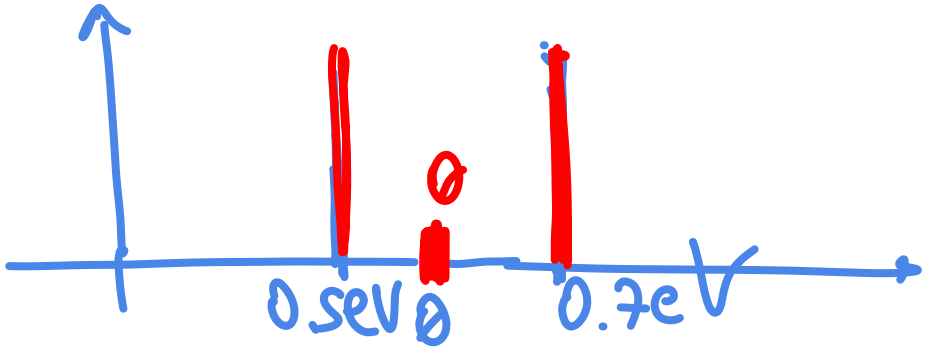
$f_S \to 1$ $f_D \to 0$
$N = 1$

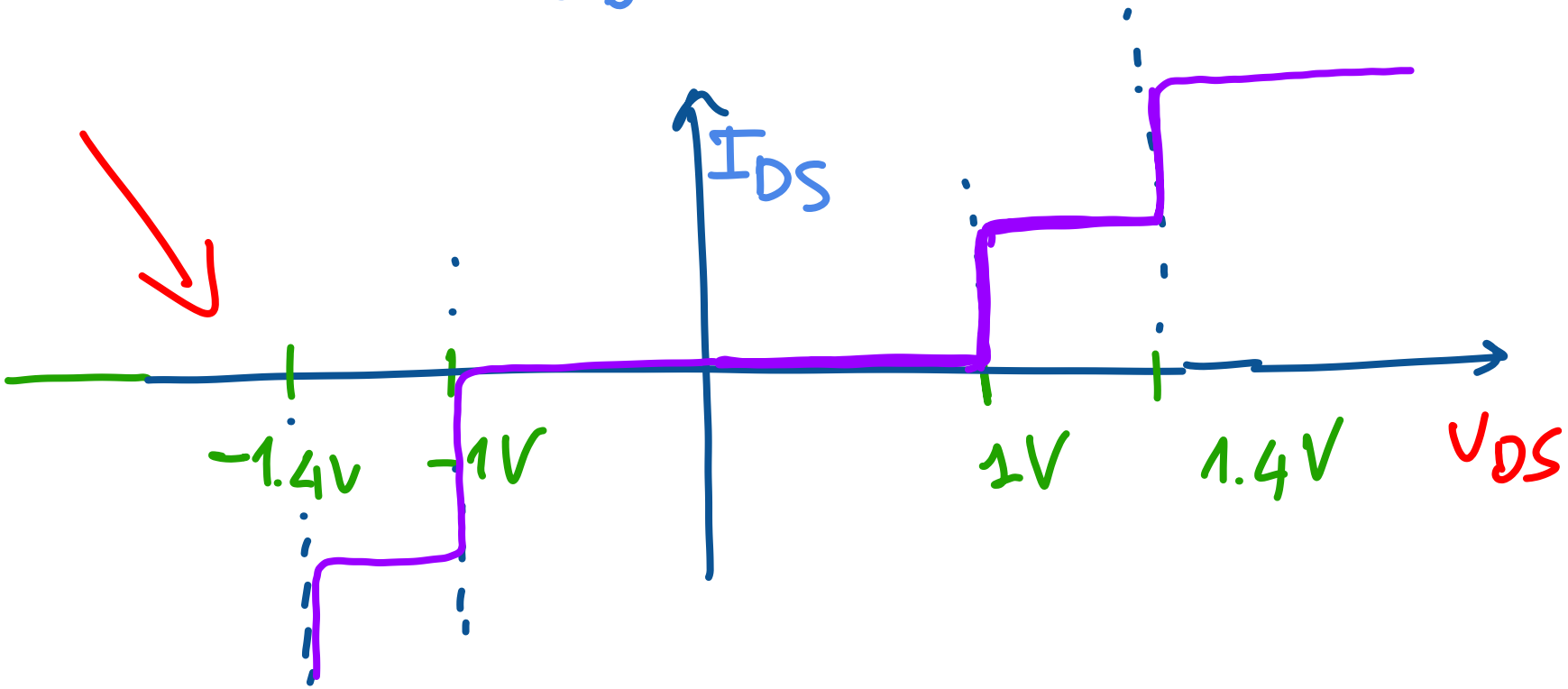
3

BENZENE DITHIOL

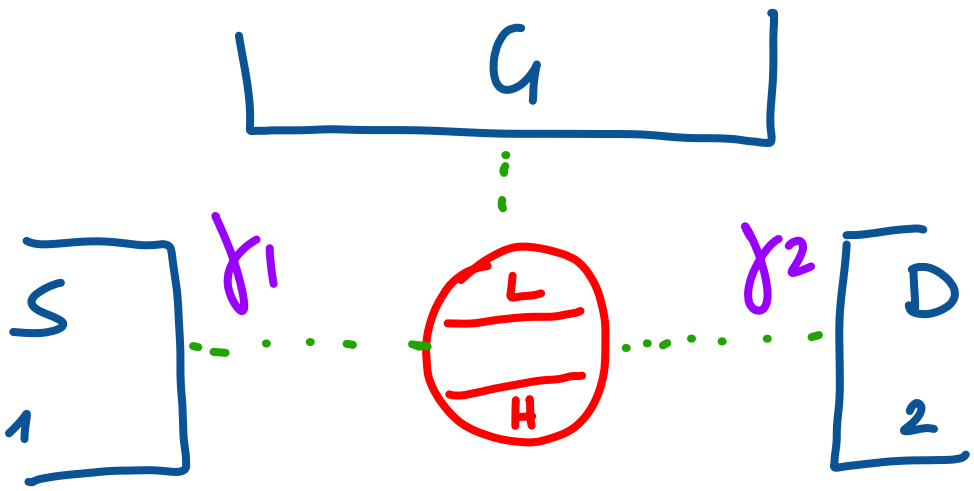


SKETCH IDS





(4)



DOT

$E_H = -5.5\,eV$

$E_L = -3.5\,eV$

@EQUILIBRIUM

$E_{F_{SYSTEM}} = -5\,eV$

STEP (A) DISCRETE LEVEL, NO C.E.

STEP (B) DISCRETE LEVEL, WITH C.E.

STEP (C) BROADENING, NO C.E

$\gamma_1 = 0.1\,eV$

$\gamma_2 = 0.1\,eV$

$C_S = C_D = 0.5\,aF$

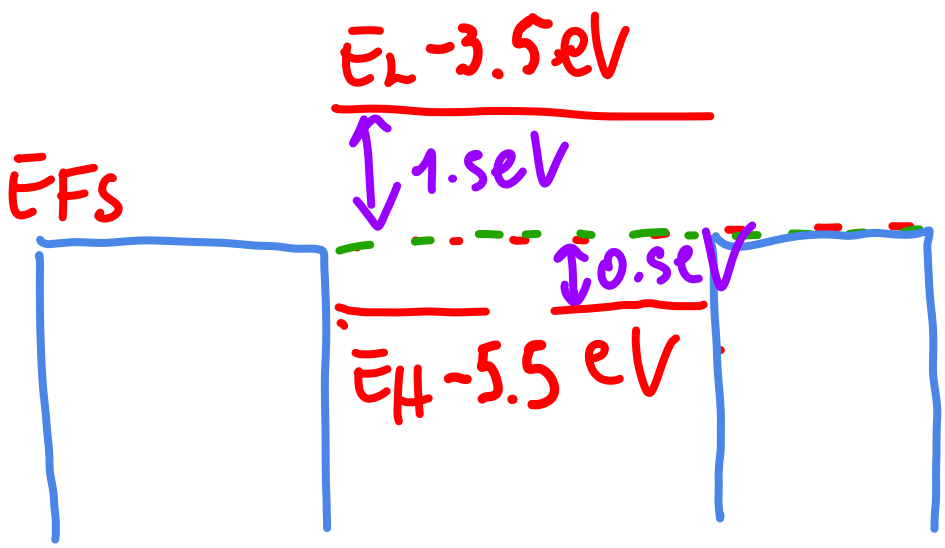
$C_G = 1\,aF$

$\forall$ STEP:

1) $I_{DS}(V_G = 0, V_{DS})$
2) $I_{DS}(V_{GS} = 1, V_{DS})$
3) $I_{DS}(V_{GS} = -1, V_{DS})$
4) $I_{DS}(V_{GS}, V_{DS} = 1)$

STEP (A) 1) 2) 3) 4)

@EQUILIBRIUM



Fermi level of the system @ EQUI associated to source

$E_{FD} = E_{FS} - q V_{DS}$

if $V_{DS} = 0V$
@EQUILIBRIUM

USING THE CAPACITIVE MODEL W/OUT C.E.

LET'S CALCULATE V_{DOT}, U_{DOT}

$$U_{DOT} = -q \frac{C_G}{C_{ES}} V_{GS} - q \frac{C_D}{C_{ES}} V_{DS}$$

$$\frac{C_G}{C_{ES}} = \frac{1\cdot 10^{-18}}{(0.5+0.5+1)\cdot 10^{-18}} = \frac{1}{2} = 0.5$$

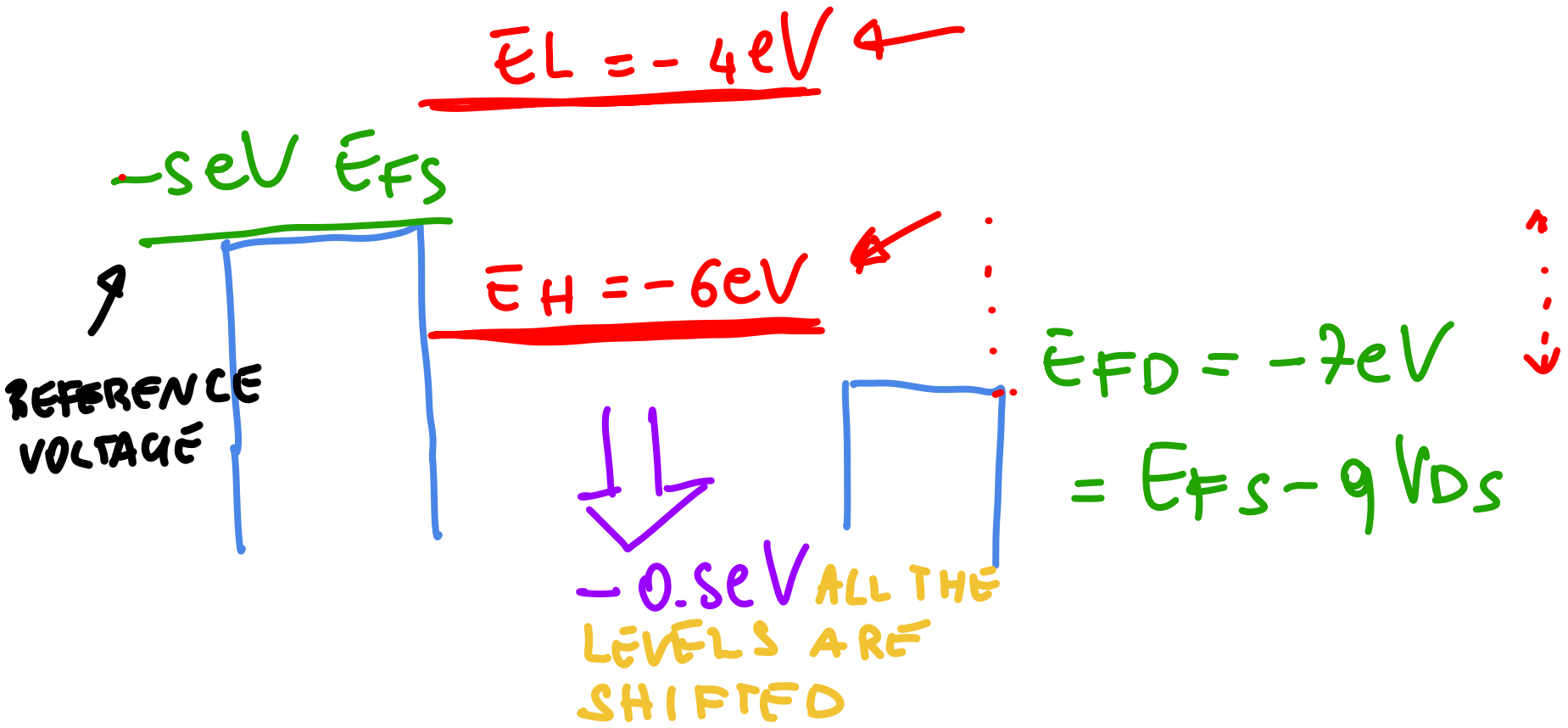
$$\frac{C_D}{C_{ES}} = \frac{0.5\cdot 10^{-18}}{2\cdot 10^{-18}} = \frac{1}{4} = 0.25$$

$$U_{DOT} = -q\ 0.5\ V_{GS} - q\ 0.25\ V_{DS}$$

case 1) $V_{GS} = 0V$ for $V_{DS} = 2V$ (to fix ideas)

$$U_{DOT} = -q \cdot 0,25 \cdot 2 = -0.5eV$$

SHIFT TOWARD NEGATIVE ENERGIES



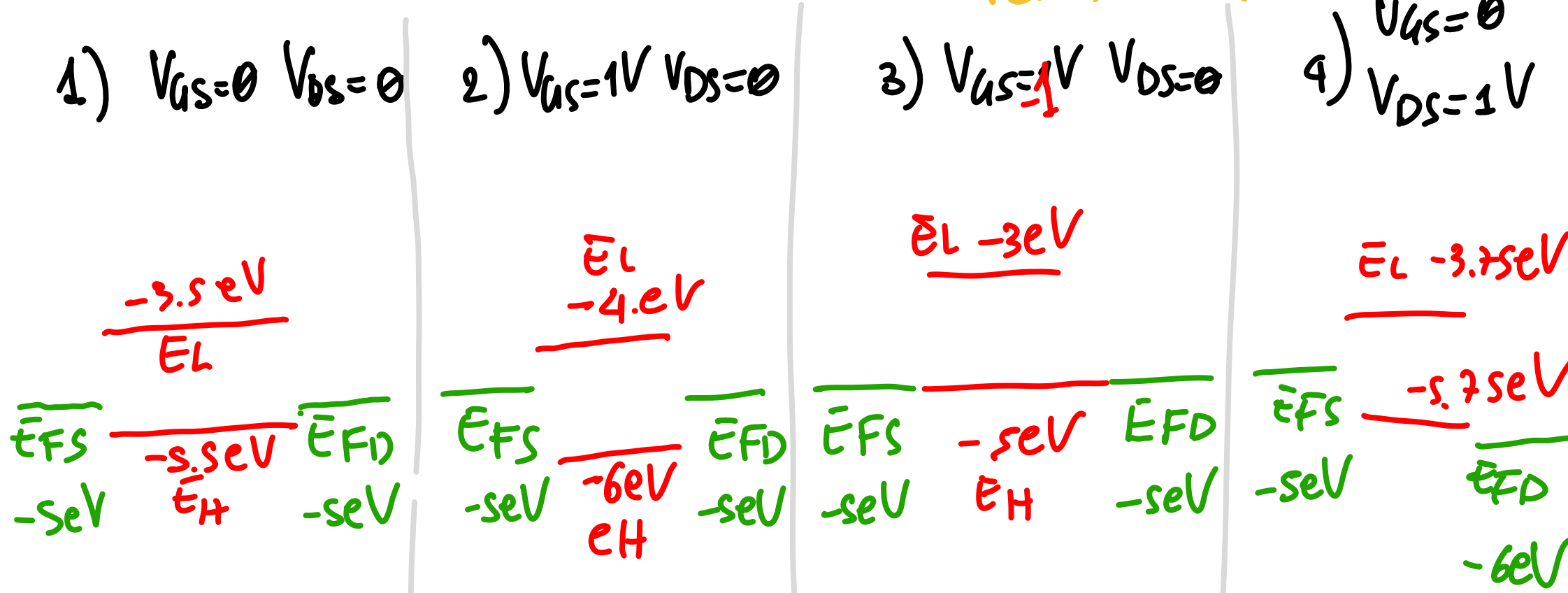
$$I_{DS} = \frac{2q}{h}\int_{-\infty}^{+\infty} T(E - V_{DOT})\left[f(E, E_{FS}) - f(E, E_{FS} - qV_{DS})\right] dE$$

TO SEE THE STARTING POINTS IN ALL CASES (*)

STEP ② 1) 2) 3) 4)

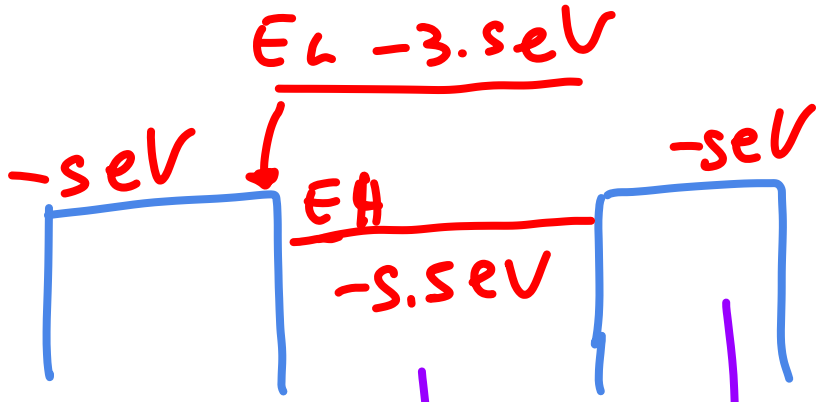
E_{FS} IS THE REFERENCE POINT AT E_F

1) $V_{GS}=0$ $V_{DS}=0$ 2) $V_{GS}=1V$ $V_{DS}=0$ 3) $V_{GS}=-1V$ $V_{DS}=0$ 4) $V_{GS}=0$ $V_{DS}=1V$



ANALYZE NOW ∀ CASE THE EVENTS WHEN V_{DS} (case a, b, c) or V_{GS} (case d) is changing, and plot the graph with values

STEP A core 1) $V_{DS} = 0V$ → $V_{DS} > 0V$



- BIAS WINDOW GROWS
- U_{DOT} ↘ $-q0.25V_{DS}$
- 1° EVENT WE EXPECT IS HOMO ENTERS IN BIAS WINDOW FOR WHICH V_{DS}?

$-qV_{DS}$

$-q\,0.25V_{DS}$

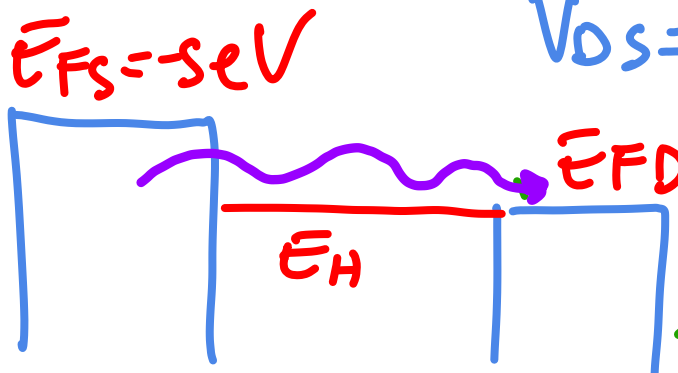
WE CALCULATE WHEN: $E_H - 0.25 \cdot X = E_{FD} - X$

$-5.5 - 0.25\,X = -5 - X$

$X \simeq 0.68\,V$

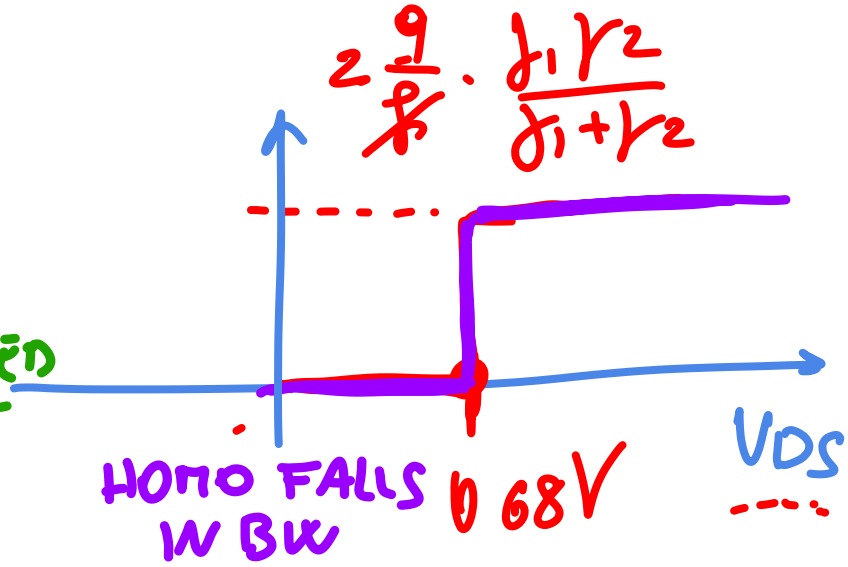
the NEW POSITION OF E_H DUE TO V_{DSX}

the NEW position OF E_{FD} DUE TO V_{DSX}



V_{DS}= 0.68V V_{GS}=0

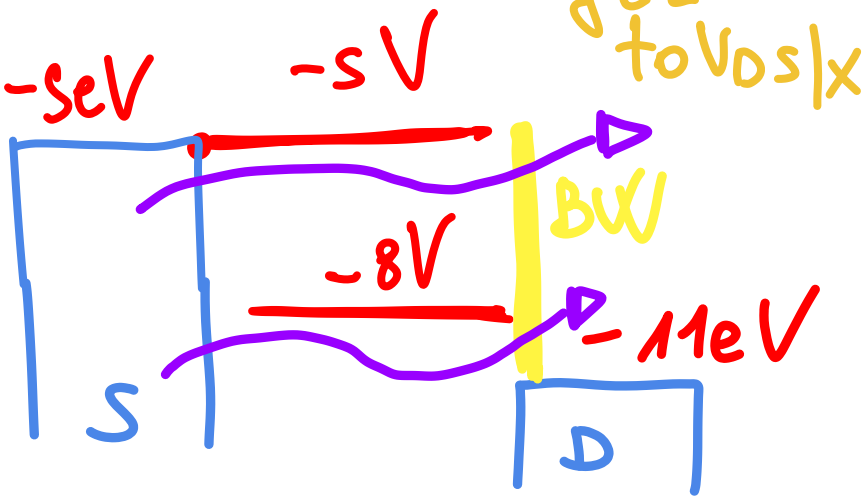
HOMO IS ALIGNED FROM THIS EVENT 1 ELECTRON CAN FLOW

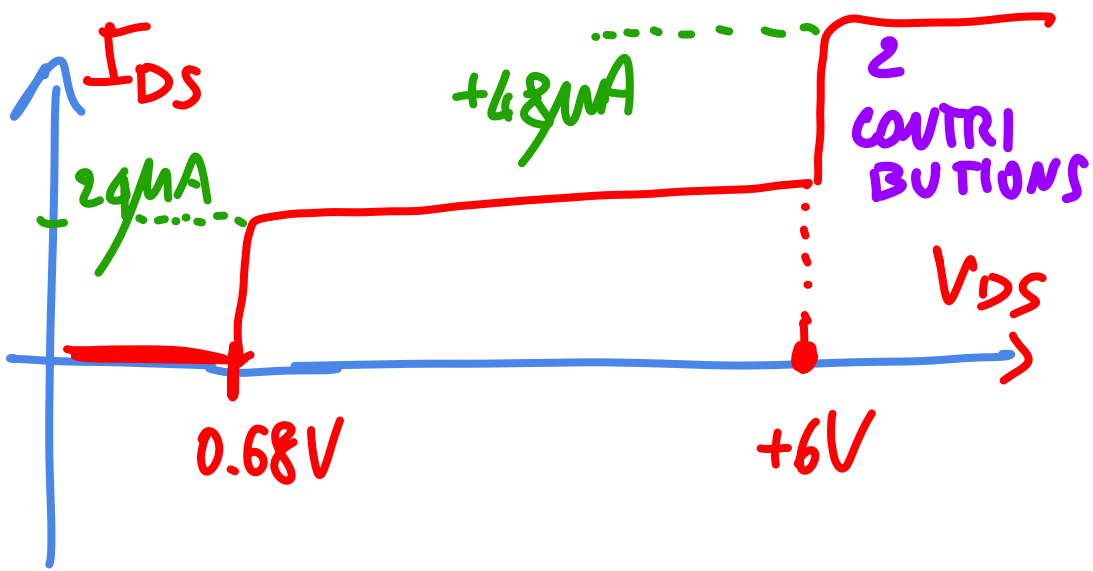


2° EVENT LUMO ⟶ BIAS WINDOW

$$E_L - q\cdot 0.25\,X = E_{FS} \qquad -3.5-\frac{X}{4}=-5 \quad X=6V$$

+ the next value of E_L due to $V_{DS}|_X$





COMPLETE FOR $V_{DS} < 0$ $E_{FD} > E_{FS}$

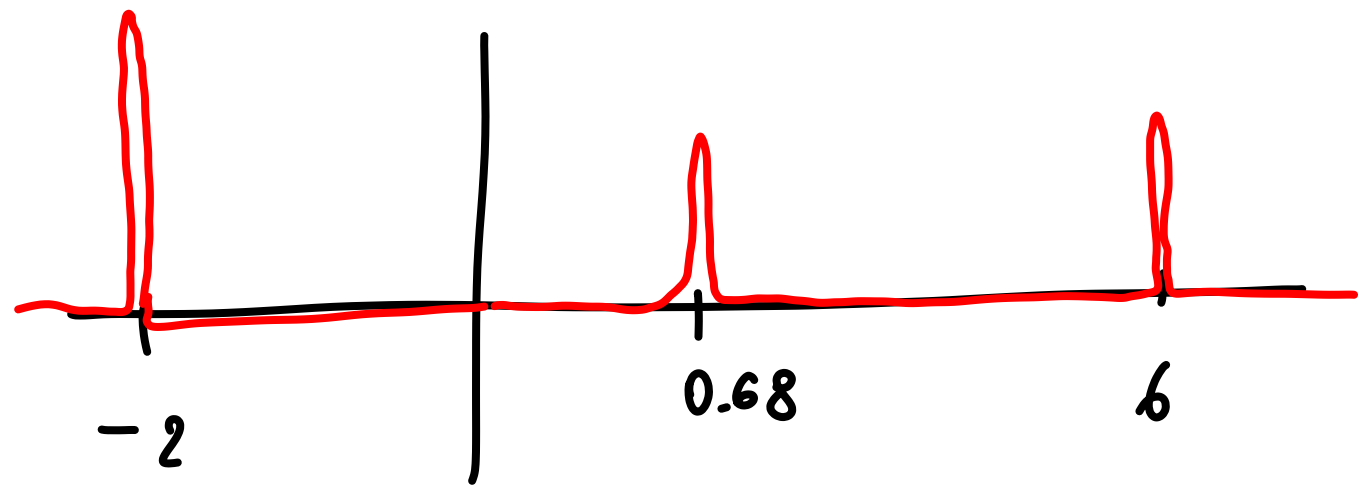
3RD EVENT — LUMO ⟶ BIAS WINDOW $V_{DS} = -2V$

4TH EVENT — HOMO ⟶ " " $V_{DS} = -2V$

⟶ HOMEWORK! calculate how -2 is derived and plot the current (CURRENT IS NEGATIVE)

DIFFERENTIAL TRANSCONDUCTANCE

$$\left| \frac{\partial I_{ds}}{\partial V_d} \right|$$



REPRESENTS THE VARIATION OF CHARGE THAT ENTERS THE CHANNEL

STEP (A) Case 1 → COMPLETE FOR ALL CASES THE CALCULATION AND PLOT I_{DS}

Case 2, 3, 4 → FROM THE STARTING RESULTS CALCULATED ALREADY see (*)

CALCULATE THE EVENTS, THE V_{DS} OR V_{GS} CAUSING THE EVENTS AND PLOT I_{DS}

In POINT 4 attention to $\frac{\partial I_{DS}}{\partial V_{GS}}$, the portion of the peaks in events are used to measure the empty of the dots

STEP (B) CHARGING EFFECT WITH DISCRETE LEVELS

DESCRIBES WHER THE DOT IS

$$\hookrightarrow U_{DOT} = -q\frac{C_a}{C_{ES}} - q\frac{C_D}{C_{ES}} + \frac{q^2(N-N_0)}{C_{ES}}$$

N_0 ELECTRONS AT EQUILIBRIUM

TO HAVE AN IDEA OF THE ORDER OF MAGNITUE HERE LET'S CALCULATE THE IMPACT IF 1 NEW CHARGE IS ADDED

$C_{ES} = 2aF$ FOR 1 MORE ELECTRON IN THE DOTS

THE SHIFT IN ENERGY IS $\frac{q\cdot 1}{C_{ES}} \Rightarrow \Delta U_{DOT} = \frac{1.6\cdot 10^{-19}}{2\cdot 10^{-18}} =$

$\frac{q^2\cdot(1)}{C_{ES}}\cdot\frac{1}{q}$ WE WANT IT IN eV $= 80\,mV$

FOCUS:
- FOR 1 LEVEL E_{HOMO}
- DISCRETE LEVELS
- NO CHARGING EFFECT

SIMPLIFIED ESPRESSION

FOR 1 LEVEL E_{HOMO}

$$T(E) = \frac{\pi \gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \cdot 2 \cdot \delta(E - E_{HOMO} - U_{DOT})$$

DISCRETE DENSITY OF STATES

DIRAC f. BECAUSE OF DISCRETE LEVEL

$$I_{DS} = \frac{2q}{h} \int \frac{\pi \gamma_1 \gamma_2}{\gamma_1 + \gamma_2} 2\,\delta(E - E_{HOMO} - U_{DOT}) \left[f(E, E_{FS}) - f(E, E_{FD}) \right] dE$$

DISCRETE LEVEL

$E - E_{HOMO} - U_{DOT} = 0 \quad E^* = E_{HOMO} + U_{DOS}$

HERE WE CAN EVALUATE THE CONTRIBUTION

$$I_{DS}\Big|_{HOMO \to BW} \simeq \frac{2q}{\hbar}\,\frac{2\pi\gamma_1\gamma_2}{\gamma_1+\gamma_2} \to 0 = 24\,\mu A$$

THE VALUE IS IN THE GRAPH

WHEN HOMO IS IN B.W.

WITH CHARGING EFFECT

CANNOT BE SOLVED IN CLOSED FORM

$$T(E - U_{DOT})$$

$$U_{DOT} = -q\frac{C_G}{C_{\Sigma}}V_{GS} - q\frac{C_D}{C_{\Sigma}}V_{DS} + \frac{q^2}{C_{\Sigma}}(N - N_0)$$

$$N = \sum_{i=1}^{n} \int_{R_i} \frac{1}{\gamma_{i1}+\gamma_{i2}}\, 2\delta\left[E - E_i - U_{DOT}\right]\left[\gamma_{i1}\left[f(E, E_{FS}) + \gamma_{i2} f(E, E_{FD})\right]\right] dE$$

ALL LEVELS

DISCRETE LEVELS D.O.S.

S. C. F.

HOW THE I/V CHARACTERISEIC CAN BE MODIFIED BY C.E.? LET'S DO IT STEP BY STEP

→ INJECT AN ELECTRON IN THE DOT

→ THIS SHIFTS THE POSITION OF THE DOT IN THE CHANNEL

→ THE ENERGY LEVEL COULD ESCAPE FROM THE BW!

↳ MUST TO BE SOLVED ITERATIVELY: SCF

↓ some pen & paper attempts follow

① In the "IDEAL" IV COURVE WE FOUND THRESHOLDS

$-2V$, $0.69V$, $+6V$ THAT ARE NOT AFFECTED BY C.E.

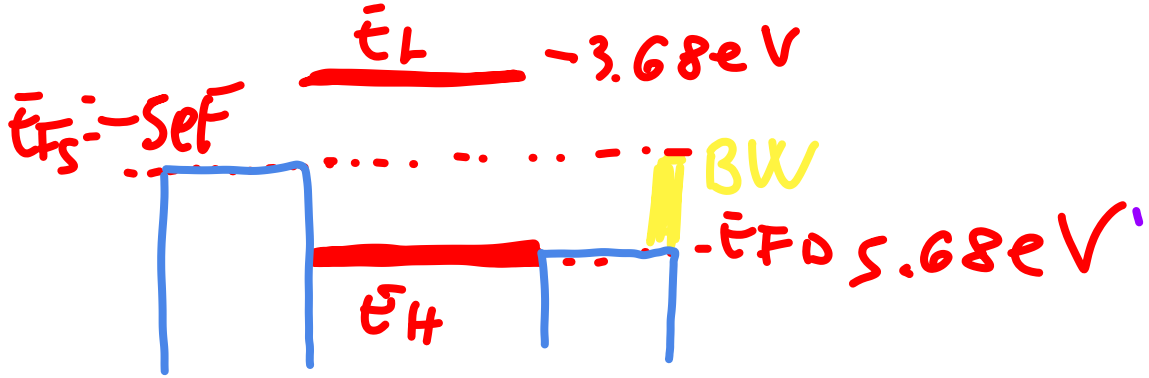
i.e : WE START TO OBSERVE THE C.E.

IMPACT ONLY WHEN THE CHARGE IS INJECTED

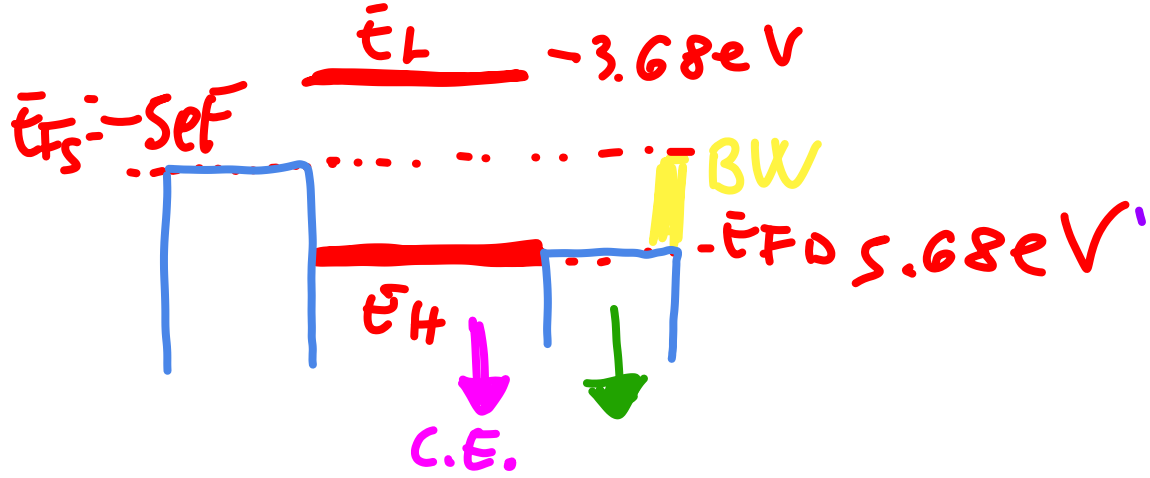
② LET'S TRY TO SEE WHAT HAPPENS NEAR THE

3 THRESHOLDS, JUST "AFTER" THE INJECTION

③ AT 0.68V



(3) AT 0.68V



THE HOMO LEVEL STATS TO CONDUCT AS IT ENTERS THE B.W.

$N_0 = 2$ (CALCULATED BEFORE)

IF $V_{DS} > 0.68$ WHAT HAPPENS TO N?

N IS $< N_0$ AND APPROXIMATELY $1 < N < 2$

BECAUSE $E_{FS} \sim 1$ and E_{FD} WAS 1

BUT IT GOES FAST $\longrightarrow 0$ WHEN DRAIN VOLTAGE IS REDUCED $\longrightarrow N \to 1$

$\Rightarrow$ $N - N_0 < 0$

[1 ÷ 2]

$\Rightarrow$ THE DOT ENERGY IS SHIFTED TO LOWER VALUES

$\Downarrow$

ELECTRONS ARE SMALLER THAN AT THE "EQUILIBRIUM"

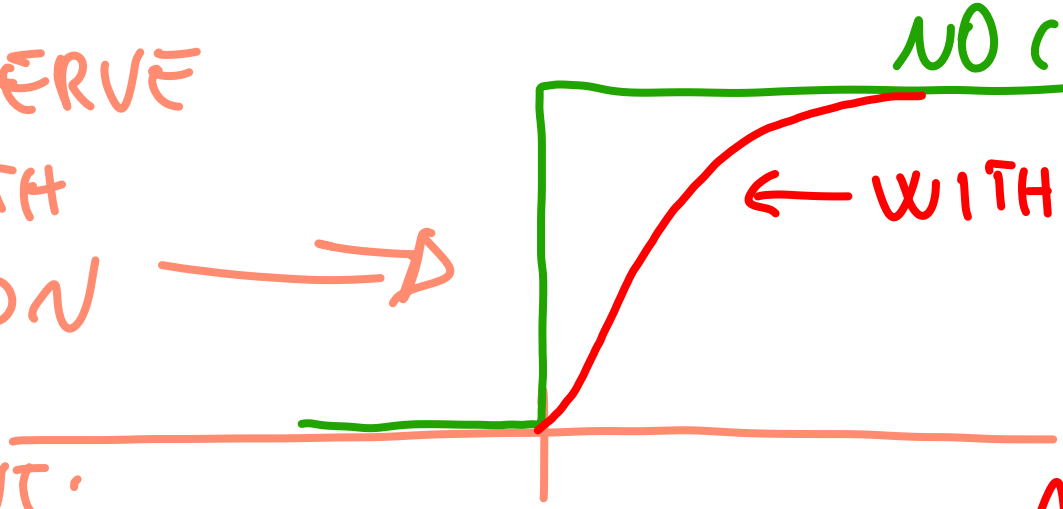
$\Rightarrow$ SO THE HOMO COULD "ESCAPE" FROM THE BIAS W.

$\Downarrow$

THE CURRENT DOES NOT INCREASE SHARPLY AS IN THE CASE WITHOUT C.E.

$\Rightarrow$ IF V_D INCREASES MORE THE "FIGHT WITH THE DOT" CONTINUES AND SOME CURRENT APPEARS....

WE OBSERVE A SMOOTH VARIATION OF CURRENT:



AS VDS INCREASES AT EACH STEP OF INCREMENT

THE STRONGER C.E. IS THE SMOOTHER THE CURRENT IS

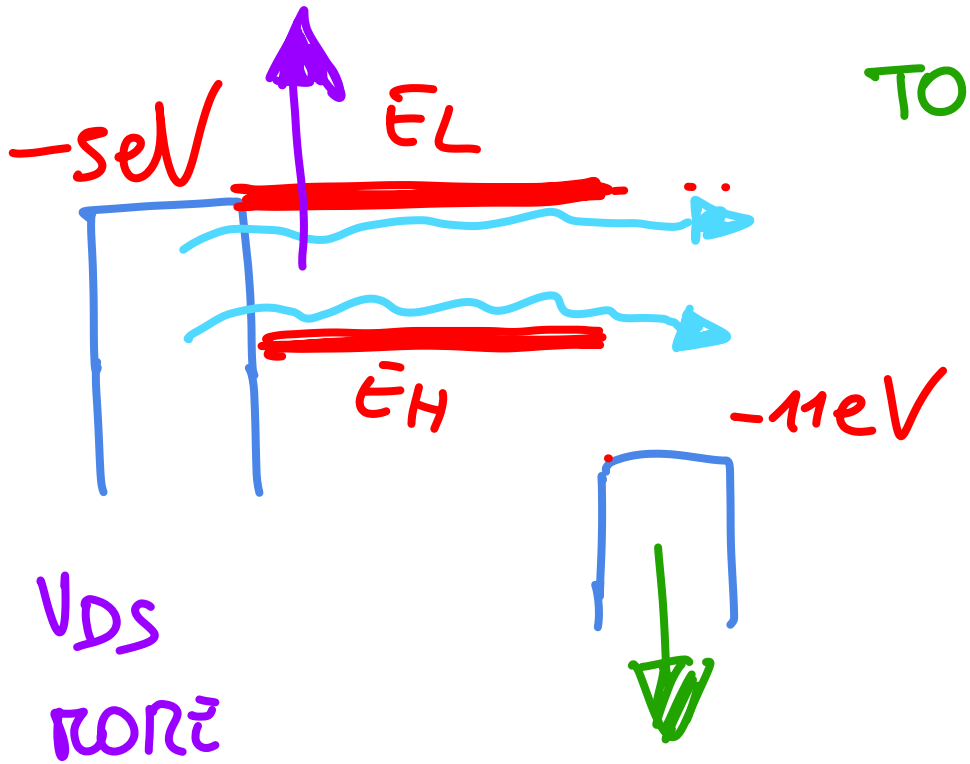
→ NEW N_0

→ NEW N

→ NEW $(N - N_0)$ THAT CAUSES DOT ESCAPE

→ $N - N_0$ REDUCES, C.E. REDUCES

④ AT $V_{DS} = 6V$ HOMO CONTINUES TO CONTRI-
BUT, LUMO STARTS
TO CONDUCT

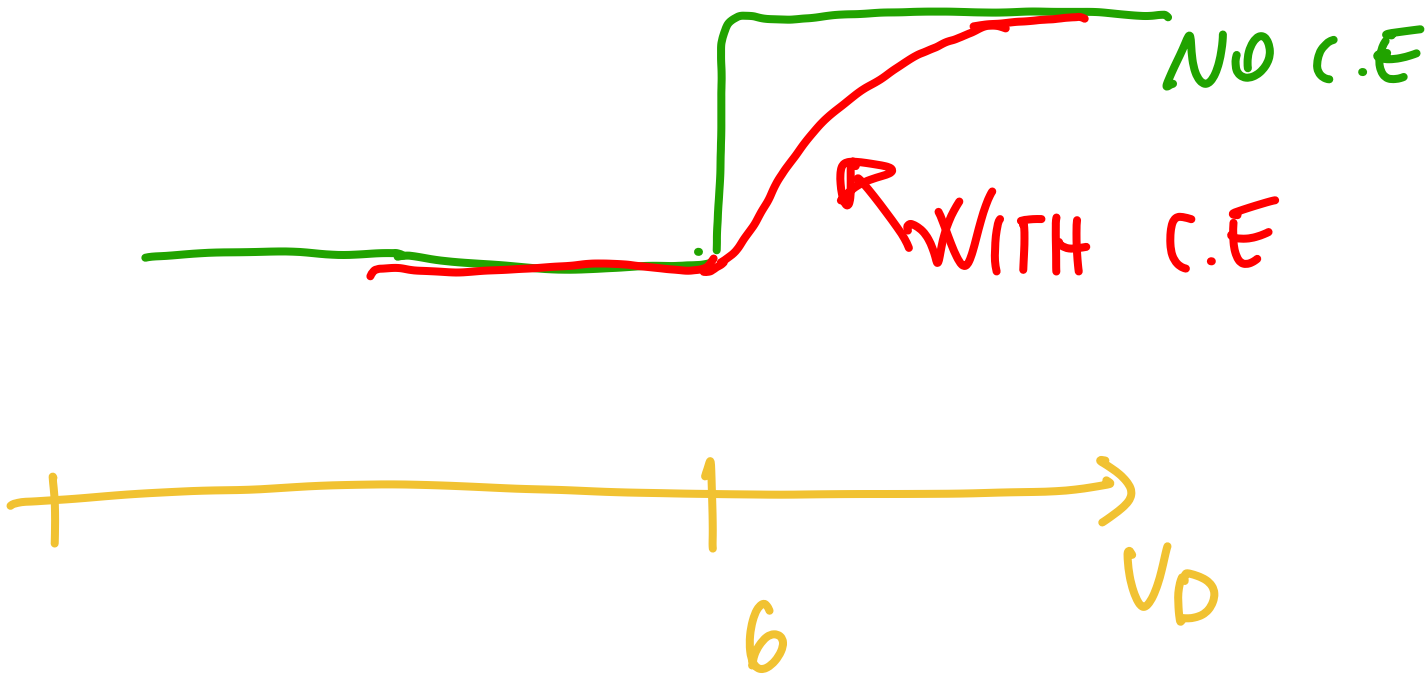


A NEW e^-
ENTERS

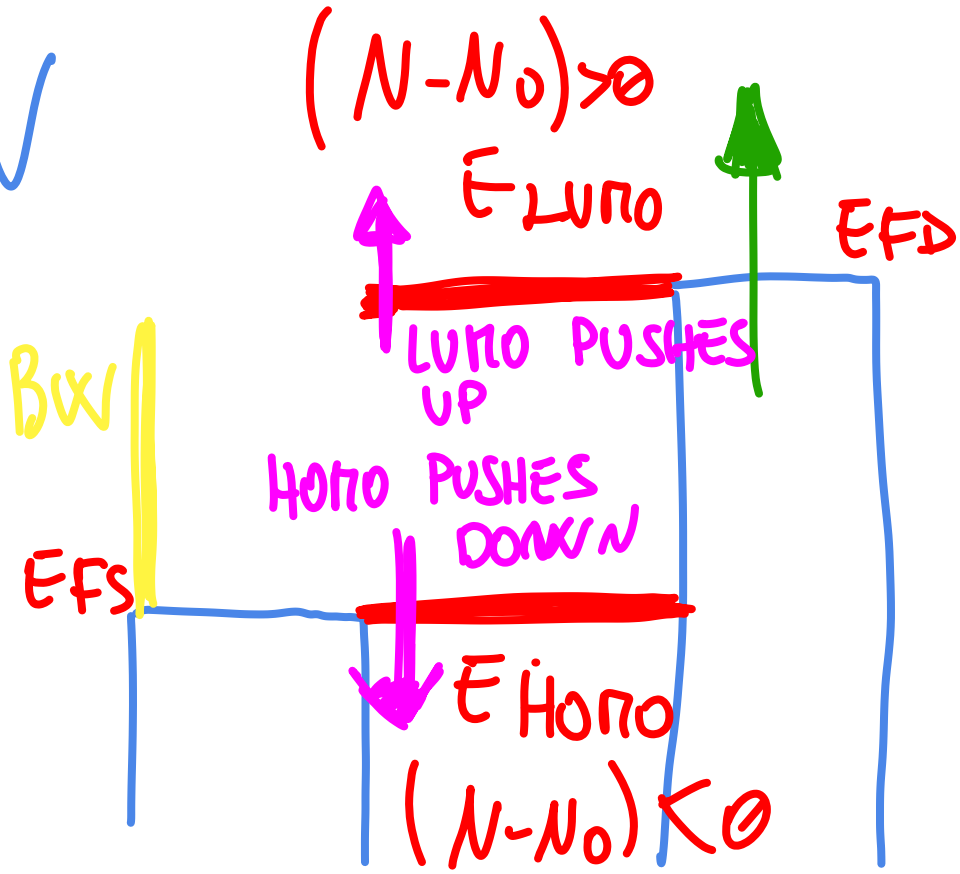
$$N - N_0 > 0$$

THE EFFECT IS
TO MOVE UP
TO HIGHER EN.
THE DOT

ONLY IF V_{DS}
INCREASES MORE
EL ENTERS MORE
IN BW, $N - N_0 > 0$
REDUCES ⇒ THE C.E.
HAS LOWER IMPACT


NO C.E
WITH C.E
6
VD

⑤ AT $V_{DS} \sim -2V$



HOMO AND LUMO START TO CONDUCT TOGETHER

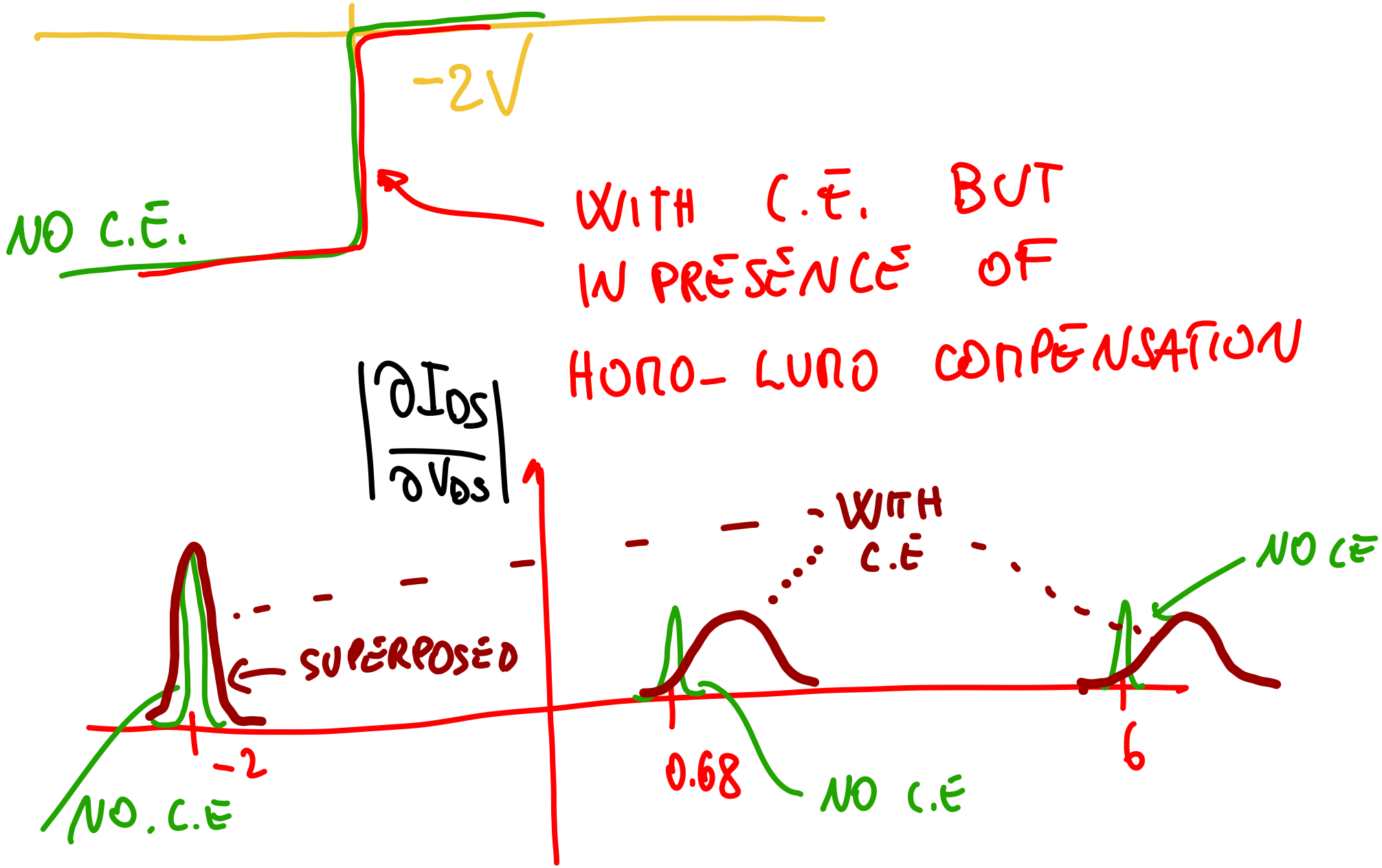
IN THE DOT WE ARE

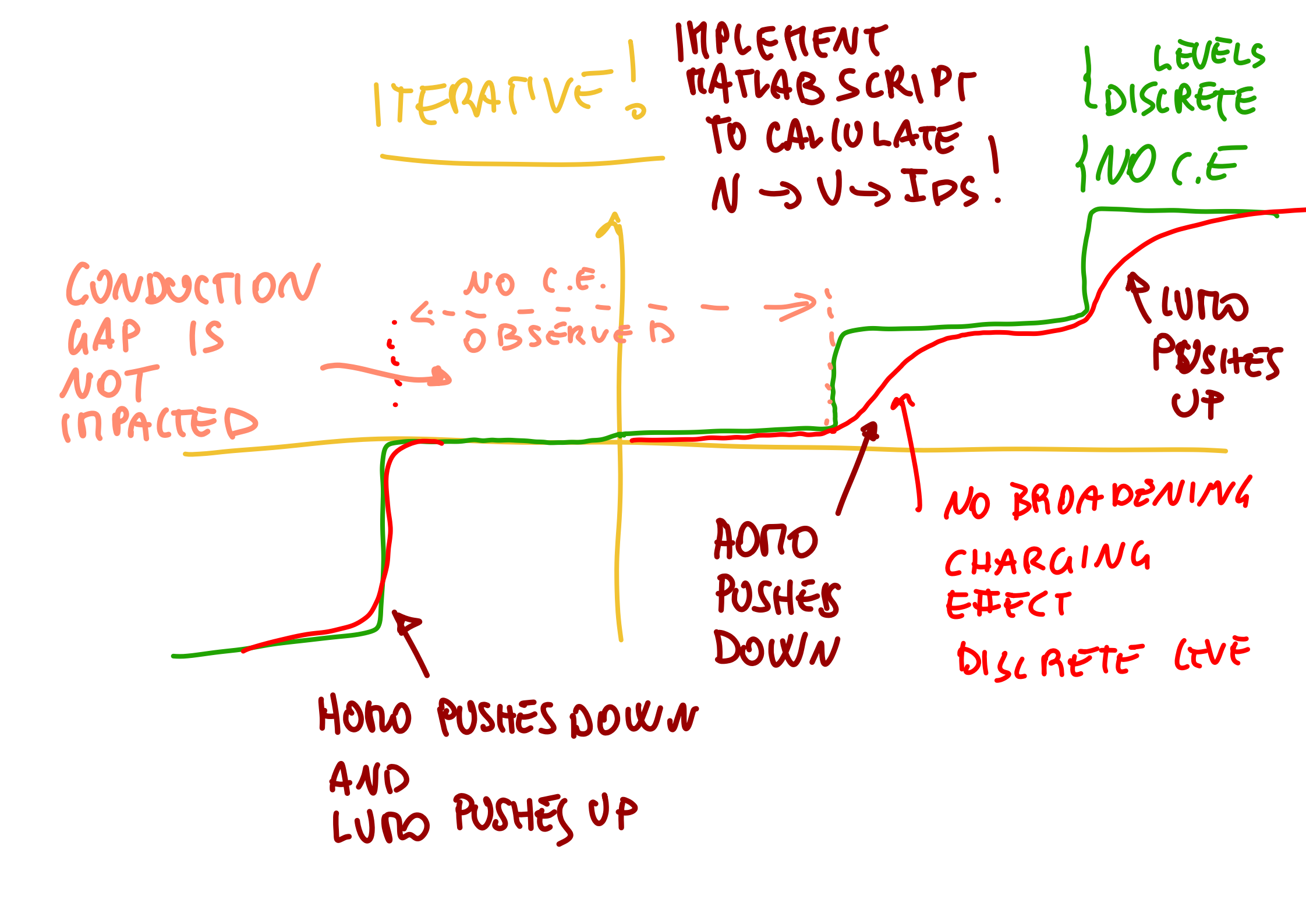
- LOOSING ELECTRONS FROM HOMO $2 \rightarrow [1 \div 2]$ (AS IN $V_{DS} \sim 0.6V$)
  - ↳ $(N-N_0)<0$
- GAINING ELECTRONS FROM LUMO (AS IN $V_{DS} \sim 6.V$)
  - ↳ $(N-N_0)>0$

] SIMULTANEUSLY / SIMMETRICAL

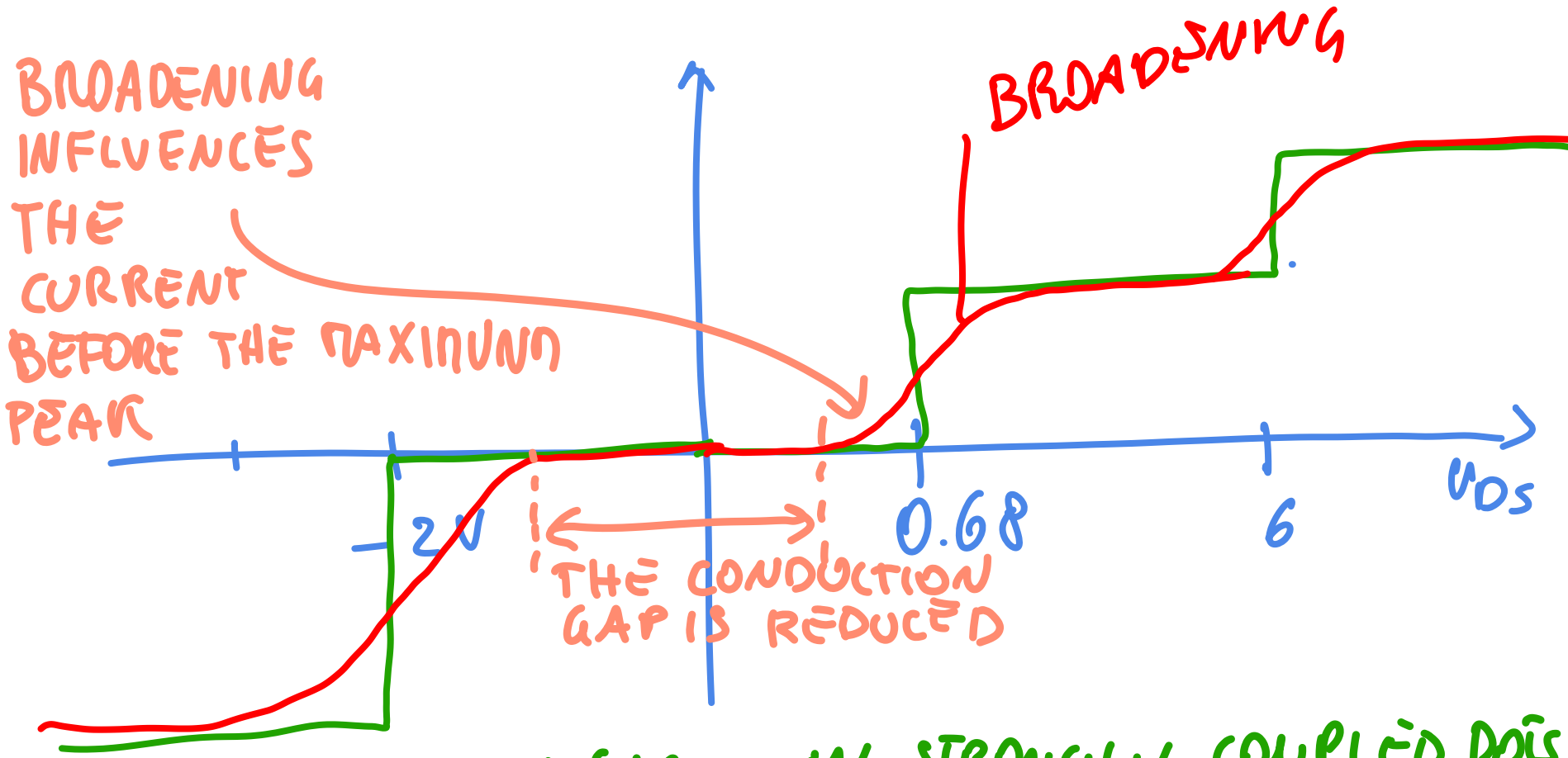
H PUSHES DOWN, L PUSHES UP ⇒ NO C.E. VISIBLE

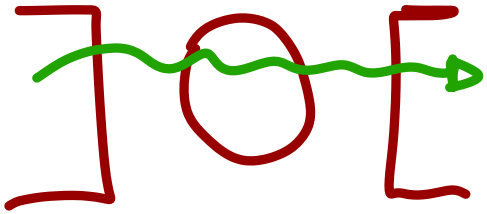
H-L: COMPENSATION

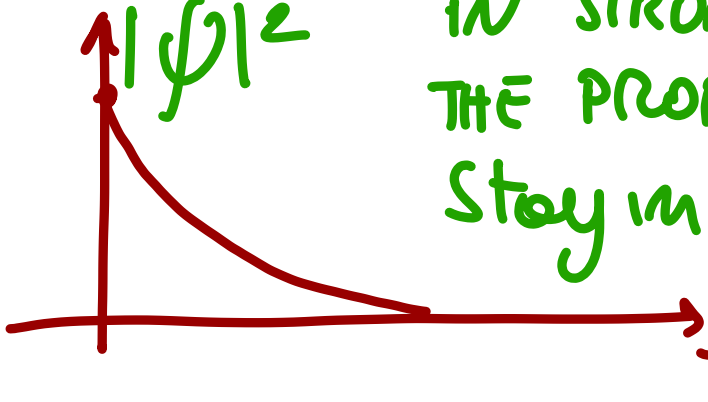

-2V
NO C.E.
WITH C.E. BUT IN PRESENCE OF HOMO-LUMO COMPENSATION
$\left|\frac{\partial I_{DS}}{\partial V_{DS}}\right|$
WITH C.E
NO CE
SUPERPOSED
-2
NO. C.E
0.68
NO C.E
6


ITERATIVE!
IMPLEMENT MATLAB SCRIPT TO CALCULATE N → U → IDS!
LEVELS DISCRETE
NO C.E
CONDUCTION GAP IS NOT IMPACTED
NO C.E. OBSERVED
LUMO PUSHES UP
HOMO PUSHES DOWN AND LUMO PUSHES UP
HOMO PUSHES DOWN
NO BROADENING CHARGING EFFECT
DISCRETE LVE

STEP (C) WITH BROADENING NO C.E







IN STRONGLY COUPLED DOTS THE PROBABILITY for é to Stay in DOTS DECAYS RAPIDLY