Quantum Transport:
Atom to Transistor

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Lecture 41a: Supplementary Topic: Coulomb Blockade

Ref. Chapter 1.5 & 3.4

Please note that this lecture overlaps with lecture 41; Hence the number 41A. The main difference is that this one includes the discussion on the origin of the General Principle of Statistical Mechanics.

Network for Computational Nanotechnology

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Review

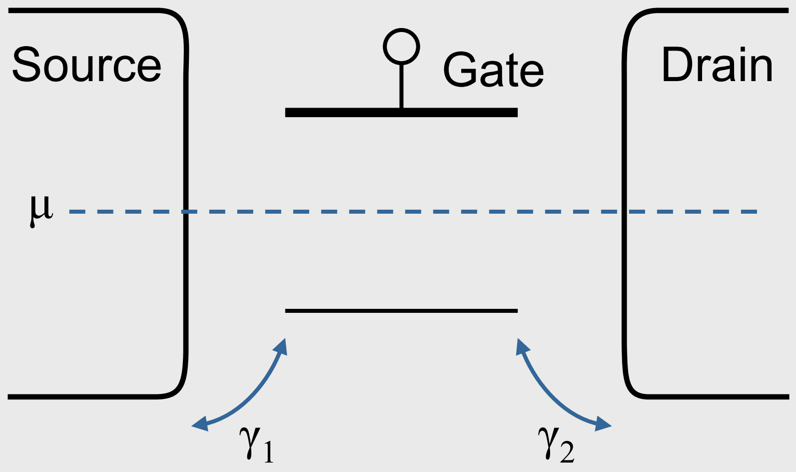
- Everything we have discussed so far has been based upon the self-consistent field picture. The self-consistent field is an approximate solution to the electron-electron interaction problem

- Over the years many self-consistent field approximations have been developed, the lowest order approximation being Poisson's equation

$$-\vec{\nabla} \cdot \left(\varepsilon \vec{\nabla} U_{\text{scf}} \right) = q^2 n$$

- Now imagine a device with only one energy level (or two spin levels) coupled to two contacts (source and drain) via γ_1 and γ_2

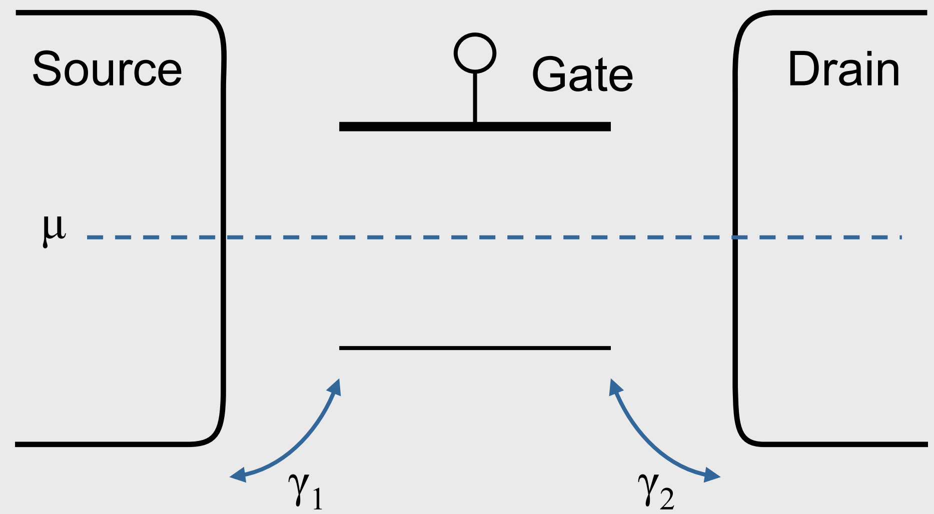
Single Level Device



Single Electron Charging

03:00

Single Level Device



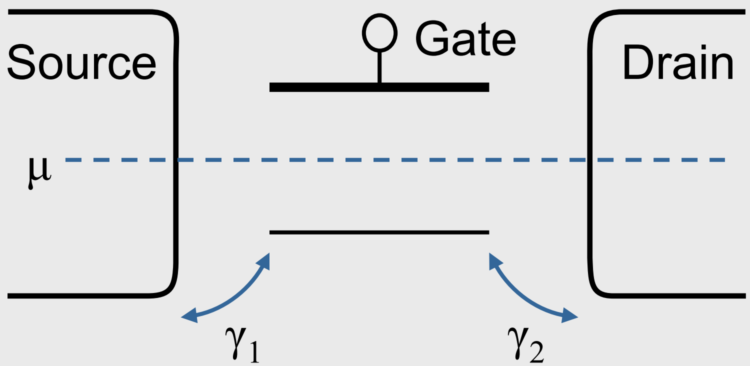
- U is very small when dealing with large structures, but for small structures, such as atoms, it can become very large. In fact U can become so large that it actually exceeds the level broadening and we call this regime Coulomb Blockade

- This device has a single electron charging energy of $U = q/C$, where C is the effective capacitance

Small *U*

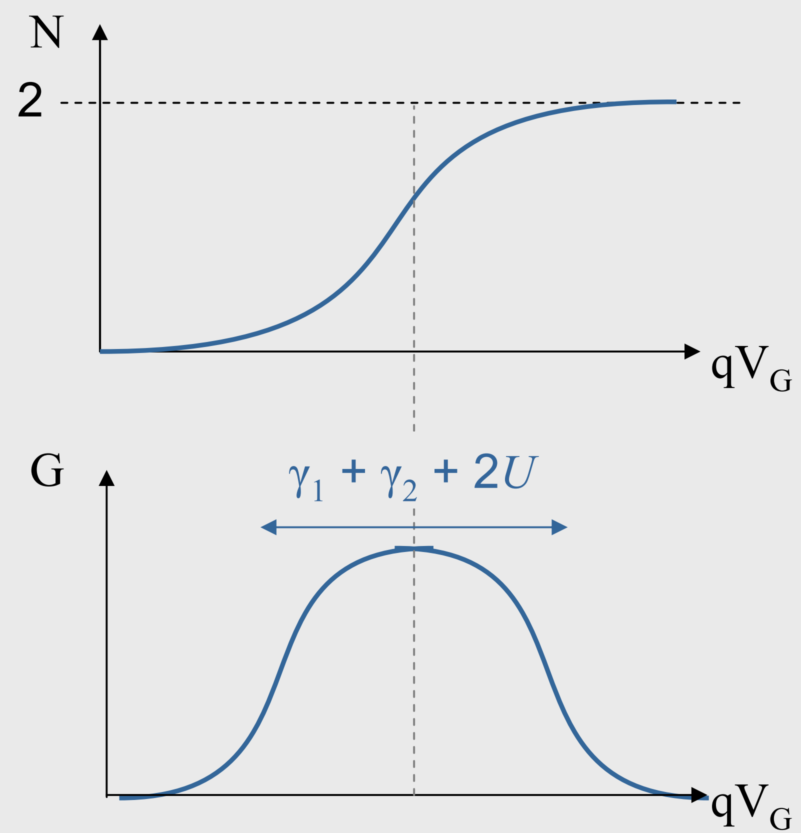
05:00

Single Level Device



- For small U the single level device gives a conduction distribution and electron count as shown on the right. *Note*: The conductance peak has a width of $\gamma_1 + \gamma_2 + 2U$, where the electron charging energy is included twice

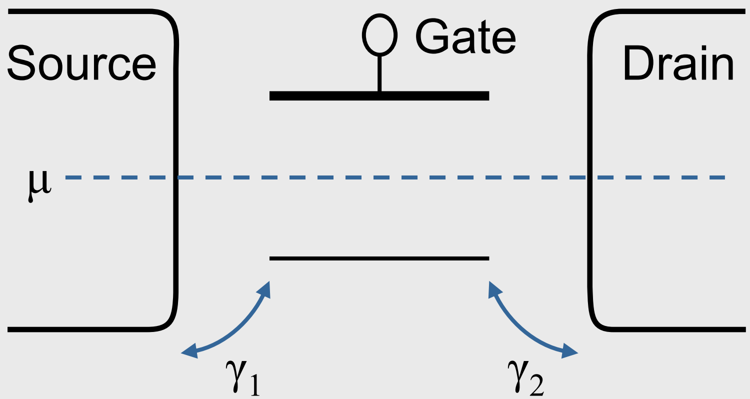
Conductance & Number of Electrons for Applied V_G (Small U)



Large U

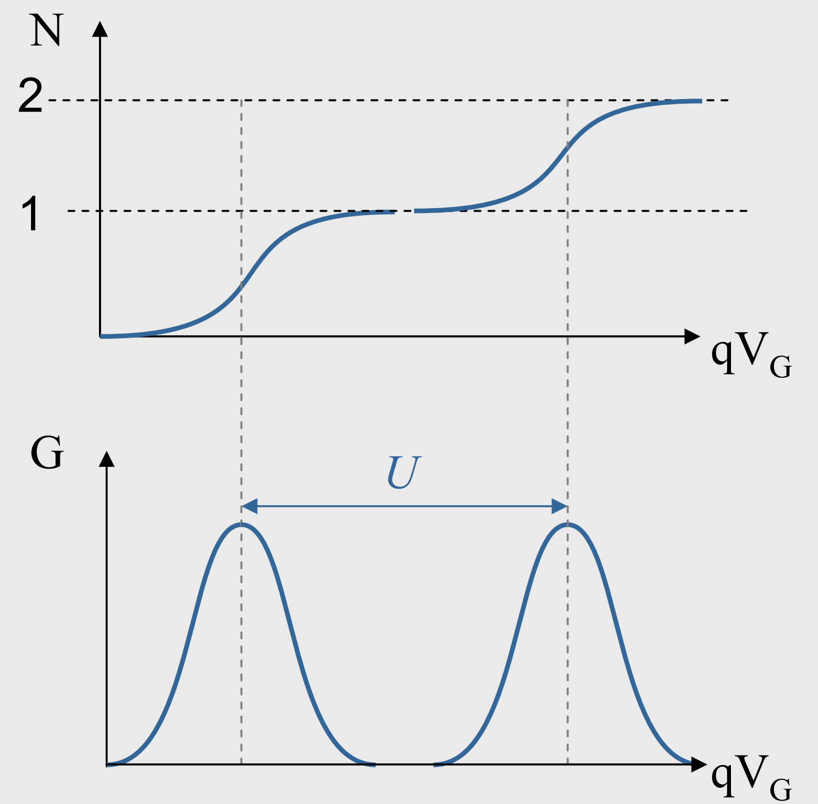
07:00

Single Level Device



- Whereas for large U, the coulomb blockade regime, we get a double peak and step for the conductance and electron count respectively

Conductance & Number of Electrons for Applied V_G (Large U)

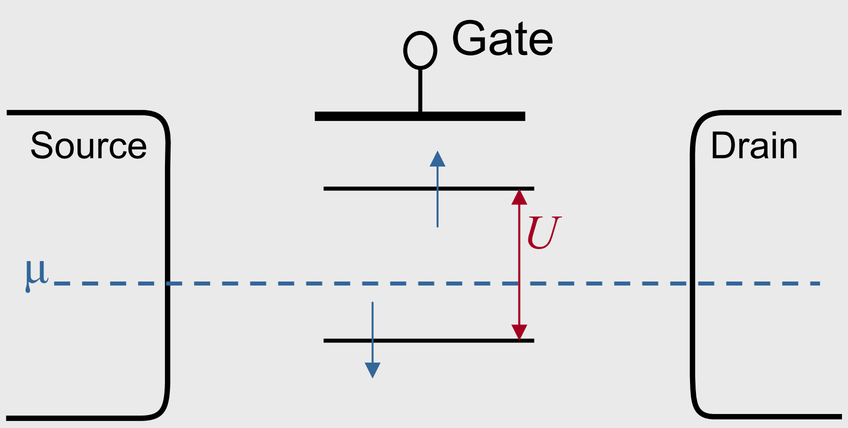


Two Levels

10:00

• Why does the coulomb blockade occur for large U? It happens because we really have two levels, rather than one level holding two electrons, a spin up and a spin down level

Spin Up and Spin Down Levels Separated by U



• For the diagram on the left, effectively the down spin level is filled first and the second electron, which will enter the up spin level, feels a charging energy of $U = q/c$. This charging energy, when large, creates an observable split in the spin levels and hence the observed coulomb blockade.

Note: The down spin only fills first for the purposes of this example; it is equally likely that the up spin level should fill first

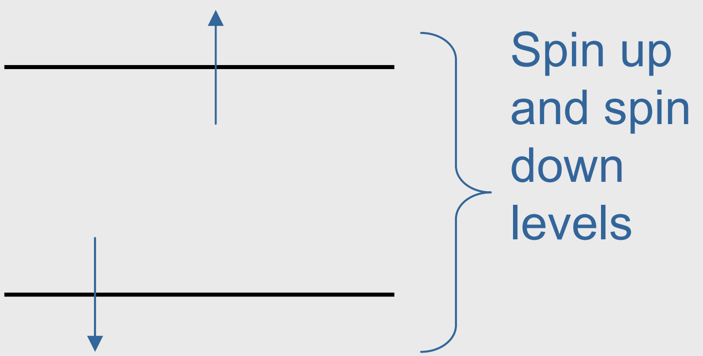
Multi-Electron Picture

11:00

- However, all of this is better explained using the multi-electron picture

- Main Idea:

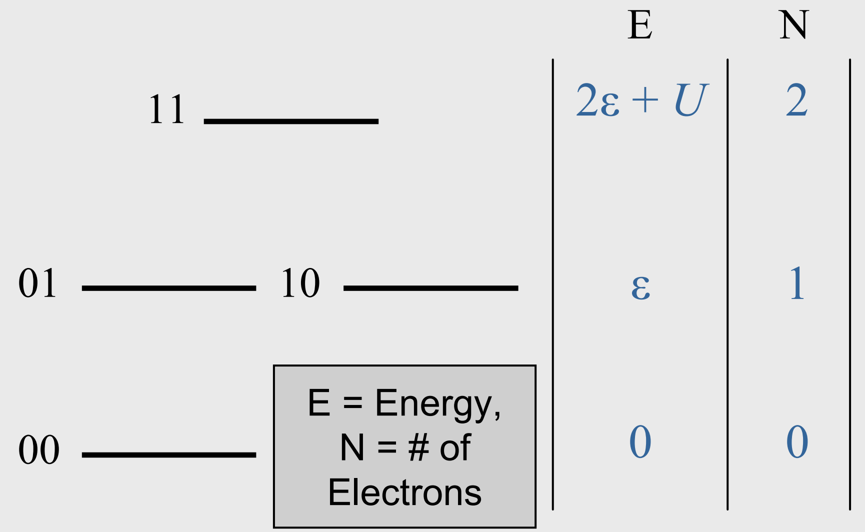
→ Let's say we have two particle levels, spin up and spin down, where each one can hold a single electron



- Main Idea Continued:

→ If we think of this as one big system, then we have 4 states with the following energies

Two Spin Level States



Applied Gate Voltage

15:00

- Now under an applied V_G the states are…

State	E	N
11	$2(\varepsilon - qV_G) + U$	2
01, 10	$\varepsilon - qV_G$	1
00	0	0

E = Energy, N = # of Electrons

- So as we apply a gate voltage the system will go from the 0 electron to a 1 electron to the 2 electron state. To describe this process we need to apply the general principle of statistical mechanics

$$P(E,N) = \frac{1}{z} e^{-(E-\mu N)/k_B T}$$

- Definition:

$$P(E,N) = \frac{1}{z} e^{-(E-\mu N)/k_B T}$$

represents the probability that the system is in a particular state with energy E and number of particles N. Note: Z is the partition function, it guarantees that the sum of all probabilities is 1

- Example:

We can show how the fermi function follows from this in a one (spin) level system

A one level system has the following probabilities for states 0 and 1…

One Level System

	E	N
1	ε	1
0	0	0

One Level System Probabilities

	E	N	P
1	ε	1	$(^1/_Z)e^{-x}$
0	0	0	$(^1/_Z)\times 1$

where $x = (\varepsilon-\mu)/k_B T$

Fermi Function

18:00

- We may calculate the partition function via the equality

$$1 = \frac{1}{z}\left(1 + e^{-x}\right)$$

$$\therefore\ z = 1 + e^{-x}$$

and the final probabilities are:

Final One Level System Probabilities

Level	E	N	P
1	ε	1	$e^{-x}/(1+e^{-x})$
0	0	0	$1/(1+e^{-x})$

- Now if we take the average of these probabilities we get

$$1 \times \frac{1}{e^{x}+1} + 0 \times \frac{1}{1+e^{-x}} = \frac{1}{1+e^{x}}$$

which is the fermi function! This result can be applied to any multi-electron system. In essence the fermi function represents the average value of P(E,N) across all electron states. The same approach applied to photons, which has no exclusion principle, leads to the Bose function

Original Problem

22:30

- Now let's return to the central problem with an additional simplification, that is, we will concern ourselves only with low temperatures such that the probability of any state being occupied is either 0 or 1. (since $k_BT \rightarrow 0$)

- So, the probability will be 1 for that state which has the minimum value of (E-μN)

- Why is this true?

Example: Take two states, the first for which

$$\frac{E-\mu N}{k_B T} = 50$$

and the second

$$\frac{E-\mu N}{k_B T} = 100$$

and since $e^{-100} << e^{-50}$,

$z = (e^{-100} + e^{-50}) \approx e^{-50}$

$\therefore P_{50} = 1$ and $P_{100} = 0$

so we see that the min(E-μN) probability dominates as ≈ 1

Filling Up States

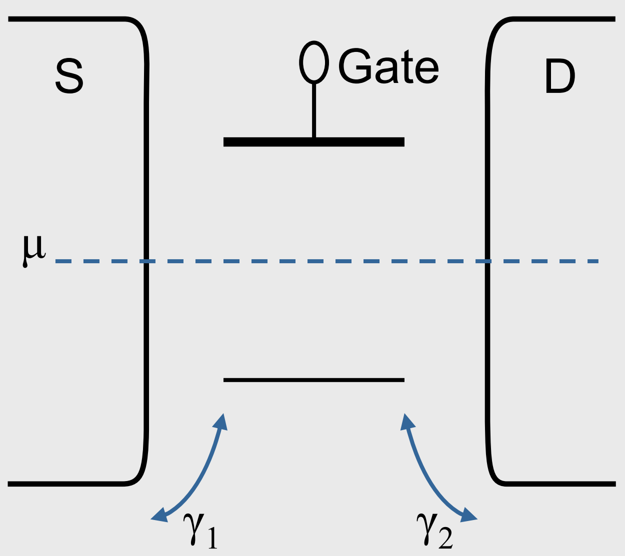
26:00

- *Main Idea*: At low temperatures we are only concerned with min(E-μN), that is the state which will be occupied
- So, for a 2-spin device, with applied V_G, the values of (E-μN) are…

- Where the device is as stated earlier…

Single Level Device

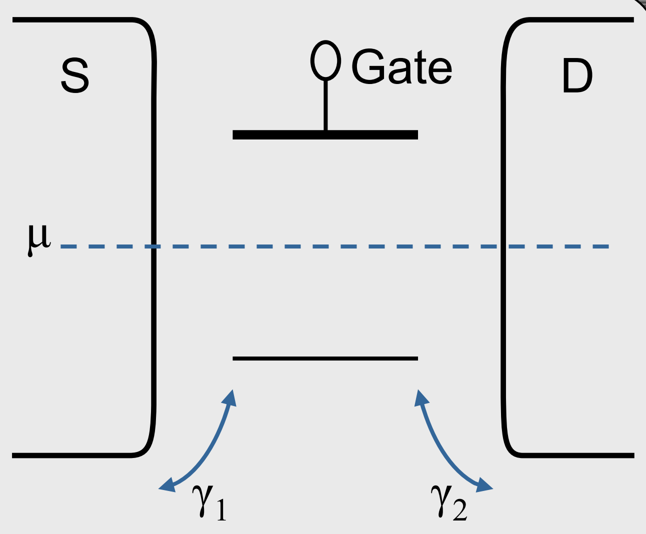
State	E	N	E-μN
11	$2(\varepsilon - qV_G) + U$	2	$2(\varepsilon - qV_G - \mu) + U$
01, 10	$\varepsilon - qV_G$	1	$\varepsilon - qV_G - \mu$
00	0	0	0



Transitions

28:00

Single Level Device



• Of course the system begins in state 00. Now, as V_G is applied, $\varepsilon\text{-}qV_G\text{-}\mu$ gets smaller and smaller. The system begins to enter the 01 and 10 states (50/50 split) at $\varepsilon\text{-}qV_G\text{-}\mu = 0$ or $qV_G = \varepsilon\text{-}\mu$

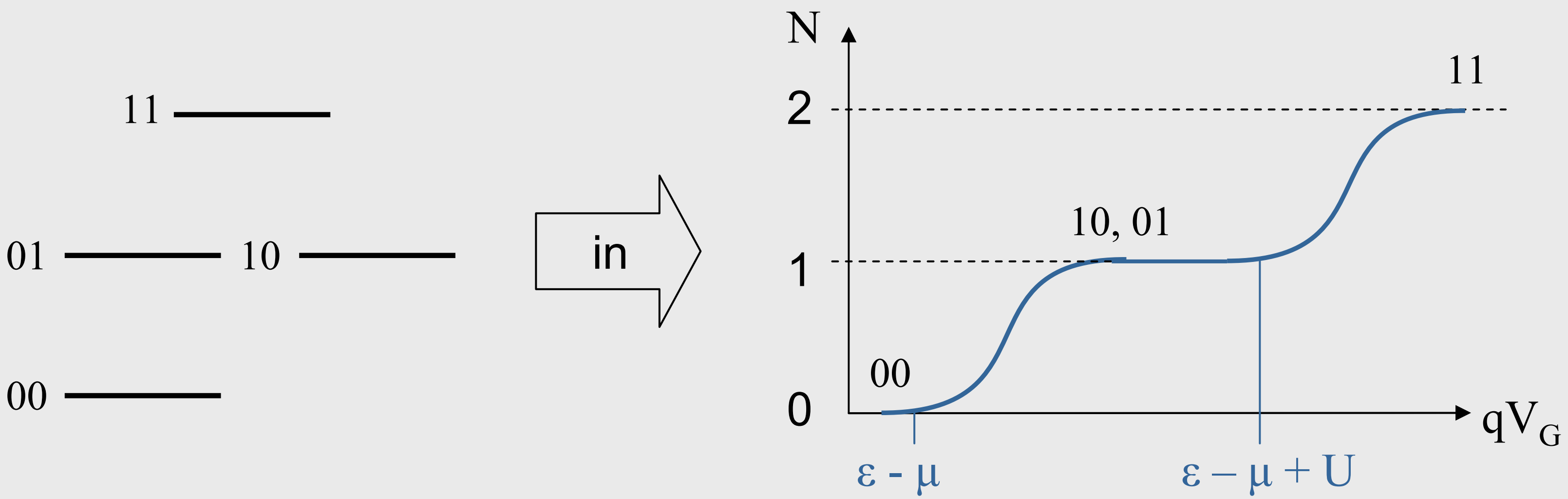
• Similarly, as we increase the gate voltage further $2(\varepsilon\text{-}qV_G\text{-}\mu)+U$ becomes even more negative at a greater rate than $(\varepsilon\text{-}qV_G\text{-}\mu)$ and begins to dominate at $2(\varepsilon\text{-}qV_G\text{-}\mu)+U = \varepsilon\text{-}qV_G\text{-}\mu$ or $qV_G = \varepsilon\text{-}\mu+U$

Multiparticle Coulomb Blockade

31:00

- *Final Picture*: we see via the multiparticle viewpoint how coulomb blockade arises:

Coulomb Blockade with Multiparticle States



- *Note*: The 00, 10, 01, 11 levels are not like single particle levels – do not confuse them (it's a full multi-electron picture)

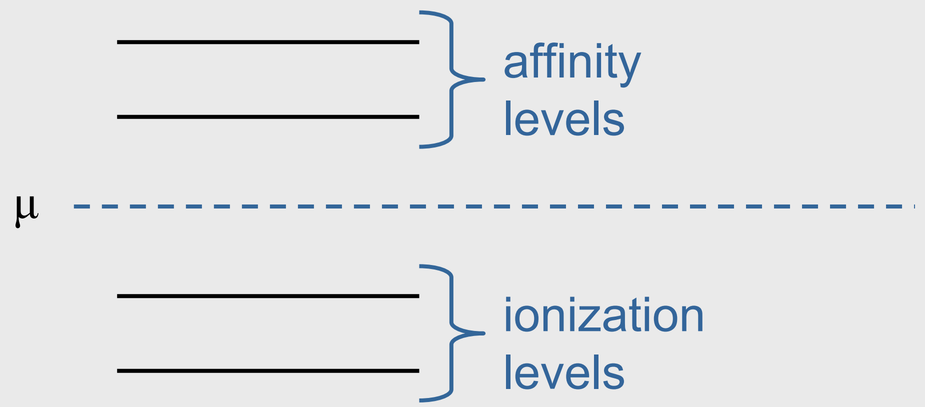
Single Particle Viewpoint

32:00

- This multi-electron picture is exact but problematic due to its size. The number of states under consideration increases exponentially, that is at 2^N, and even with 12 electrons we have well over 1000 states to consider

- Often it is difficult to get a good intuitive feeling out of the multi-electron picture, that's why we use the single electron picture

Single Electron Picture

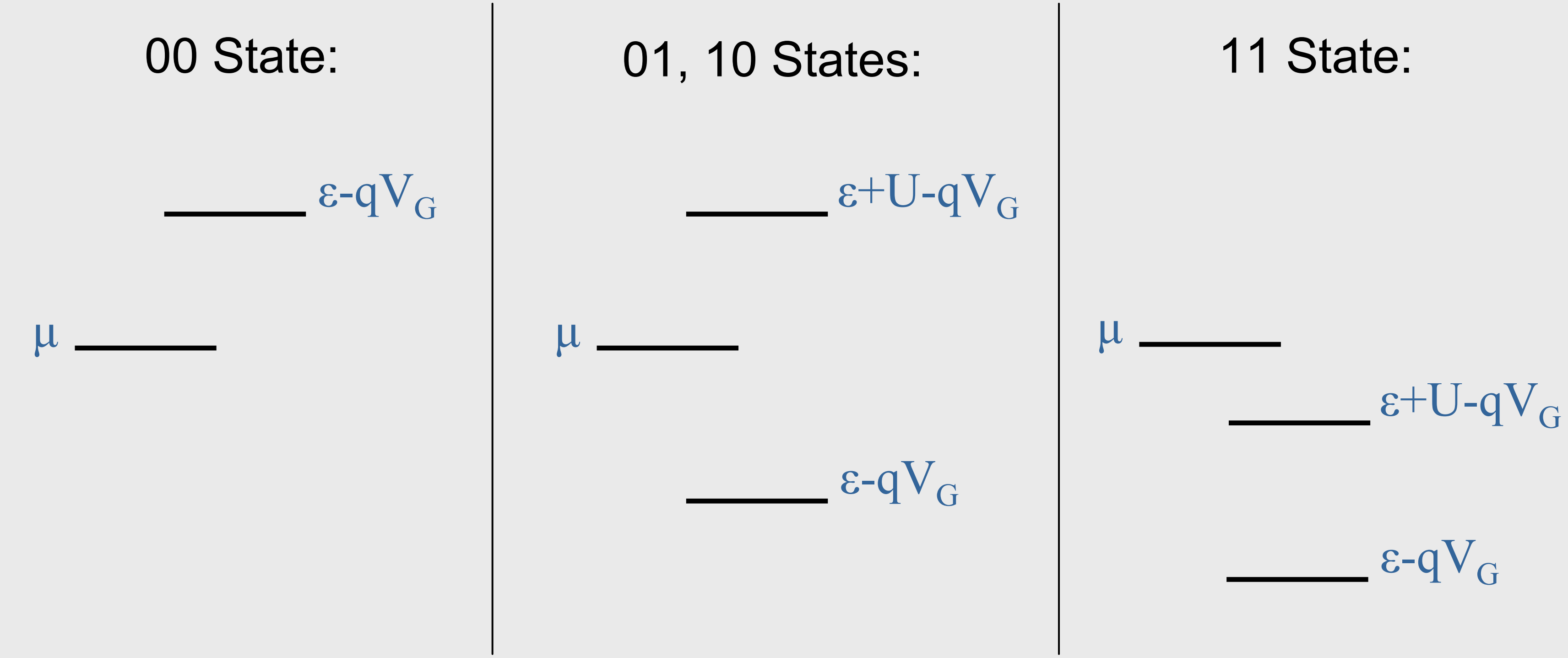


- Because the single electron picture is based upon experimental evidence it can be used in cases where it is either impossible or impractical to apply the multi-electron picture

Relating Two Pictures

36:00

• The multi-electron picture has an equivalent single electron picture for each non-degenerate state. For the 2-spin levels this means 3 single electron pictures from the multiparticle picture…



- *Next*: Where does

$$P(E,N) = \frac{1}{z} e^{-(E-\mu N)/k_B T}$$

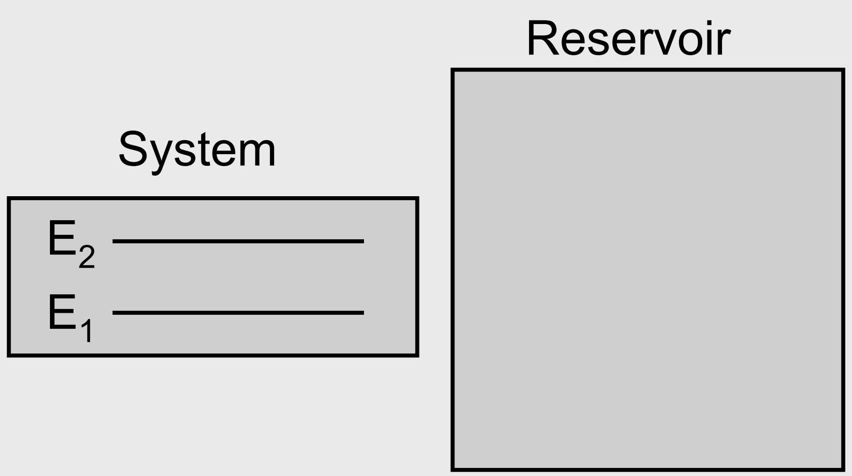
come from?

- Consider its meaning, this equation states that if you have a system in equilibrium with a reservoir then the probability that it will be in a particular state is proportional to $e^{-E/k_B T}$

- For instance the two level system below gives

$$\frac{P_1}{P_2} \alpha \frac{e^{-E_1/k_B T}}{e^{-E_2/k_B T}}$$

Two Level System with Reservoir



Reservoir DOS

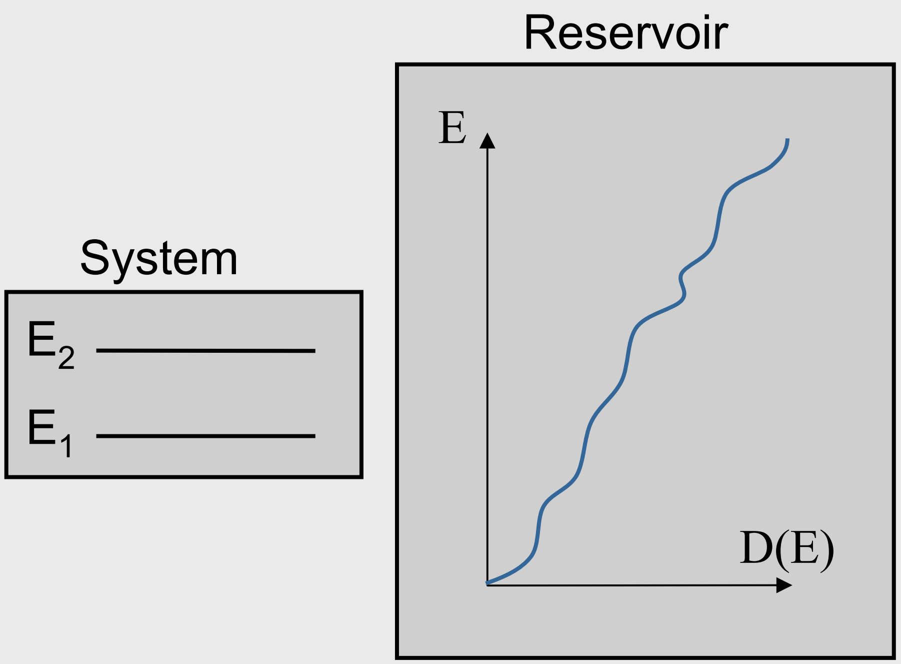
40:00

- Now, the system wants to go to the lowest possible energy (lower energy states are more probable)

- Why is this?

Basic Idea: If you have a large reservoir you can think of it as possessing some continuous Density of States (DOS). As well, view the reservoir DOS and the attached system as one big system

Reservoir DOS



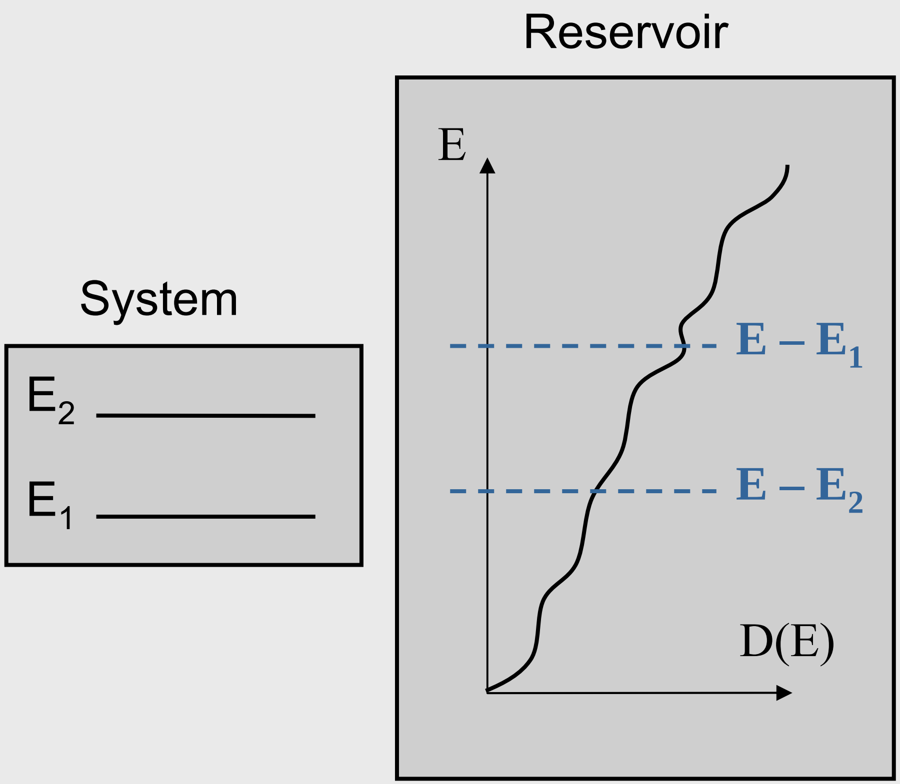
Increasing DOS

43:00

- *Basic Idea Cont'd*: So if the system is at E_1 then the reservoir is at some energy $E-E_1$ and similarly for E_2 it would be at $E-E_2$. But from the point of view of the reservoir E_1 is much more likely because it has a higher DOS than E_2!

- *Problem*: How do we know that the DOS is an increasing function of E?

Reservoir DOS



Why an Increasing DOS?

45:00

- Why do we have the DOS as an increasing function of E?

- Let's assume with energy proportional to a distribution of the type $\hbar^2k^2/2m$ (reasonable for most solids). Thus for one, two, and three dimensions the number of electron states available is proportional to $E^{½}$, E^1 and $E^{3/2}$ respectively

- And in general for n degrees of freedom the number of states available is

$N_T = CE^{n/2}$ (c is a constant).

We take the derivative to get the DOS

$$D(E) = cE^{n/2-1} \approx cE^{n/2}$$

for large n. Thus,

$$D(E) = cE^{n/2} = c\ \exp(n/2\ \ln\ E)$$

and the DOS is shown to be an increasing function of E

Probability Ratio

47:00

- From the DOS we can derive P_1/P_2 since

$$\frac{D(E-E_1)}{D(E-E_2)} = \frac{P_1}{P_2}$$

- Taylor expand D(E) about E_0 (an energy between E_1 and E_2)

$$D(E) \approx c \ \exp\left(\frac{n}{2}\ln E_0 + \frac{n}{2E_0}(E-E_0)\right)$$

$$\therefore \frac{D(E-E_1)}{D(E-E_2)} = \exp\left(\frac{n}{2E_0}(E_2-E_1)\right) = \frac{P_1}{P_2}$$

- Recall, E is the energy of the reservoir and n is the number of degrees of freedom, thus $n/(2E_0)$ represents ½ the inverse average energy per degree of freedom. But from statistical mechanics we know that the average energy per degree of freedom is $\frac{1}{2}k_BT$

Closing Comments

49:00

- Hence $E_0/n = \frac{1}{2}k_BT$ and

$$\frac{P_1}{P_2} = \exp\left(\frac{(E_2 - E_1)}{k_BT}\right)$$

so we see the basis for the P(E,N) and the fermi function. Furthermore, this shows that the complexity and size of a system does not affect the probability of states. It is a property of the reservoir, the statistical model is valid even for one level

Next Lecture: Spin