Section 12

Occupation of States

12.2 Derivation of Fermi-Dirac Statistics

Gerhard Klimeck
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School of Electrical and
Computer Engineering

Section 12
Occupation of States

One Video Segment

- 12.1 Rules of filling electronic states
  - » Pauli exclusion
  - » Total particle conservation
  - » Total energy conservation

One Video Segment

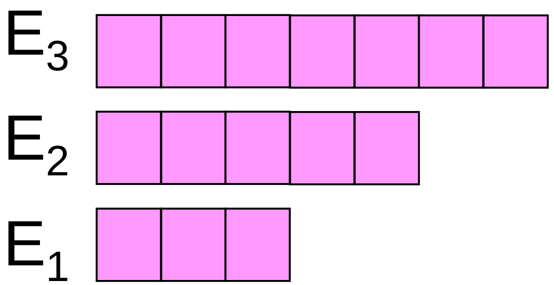
- 12.2 Derivation of Fermi-Dirac Statistics: three techniques
  - » Microcanonical ensemble - statistics
  - » Detailed Balance – thermal equilibrium & Pauli exclusion
  - » Partition Function – statistical mechanics

One Video Segment

- 12.3 Intrinsic carrier concentration

Carrier number =
Number of states x ***filling factor***

status



Reference: Vol. 6, Ch. 4

Ensemble of 3 Energy Levels

Particle conservation

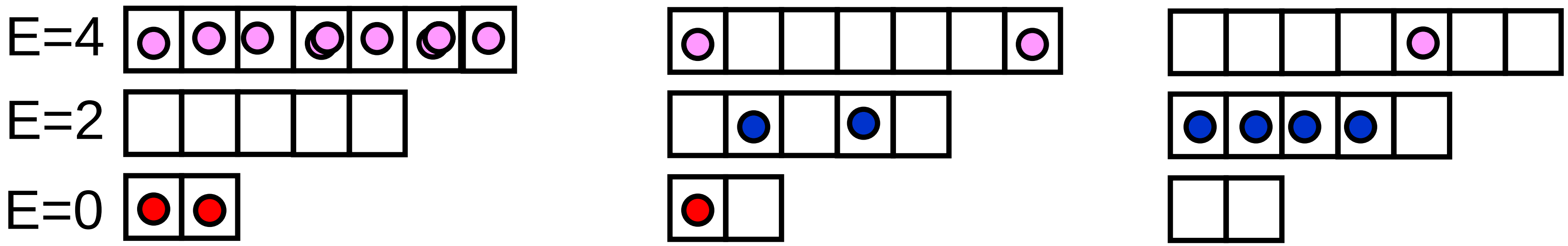
$$N_T = \sum_i N_i$$

N_T=5

Energy conservation

$$E_T = \sum_i E_i N_i$$

E_T=12

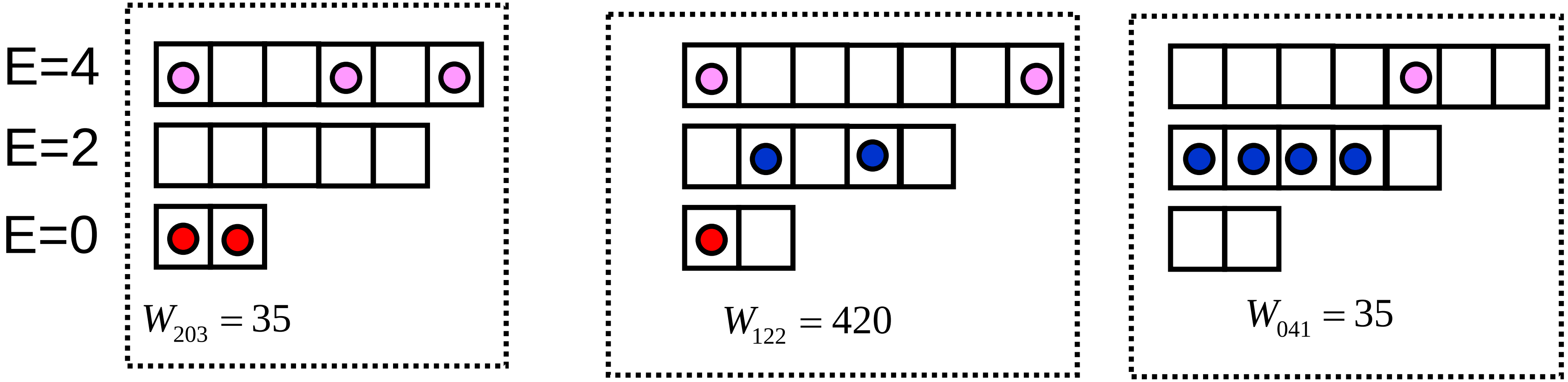


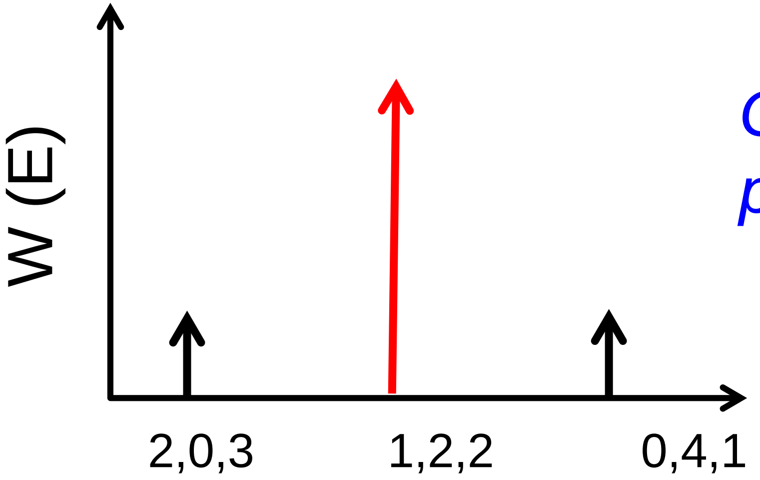
$$W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!}$$
$$= 35$$

$$W_{122} = \frac{2!}{1!1!} \bullet \frac{5!}{2!3!} \bullet \frac{7!}{5!2!}$$
$$= 420$$

$$W_{041} = \frac{2!}{0!2!} \bullet \frac{5!}{4!1!} \bullet \frac{7!}{6!1!}$$
$$= 35$$

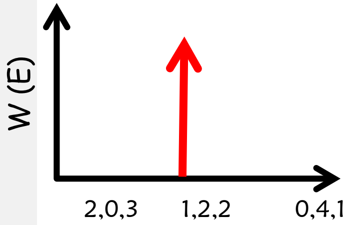
Occupation Statistics

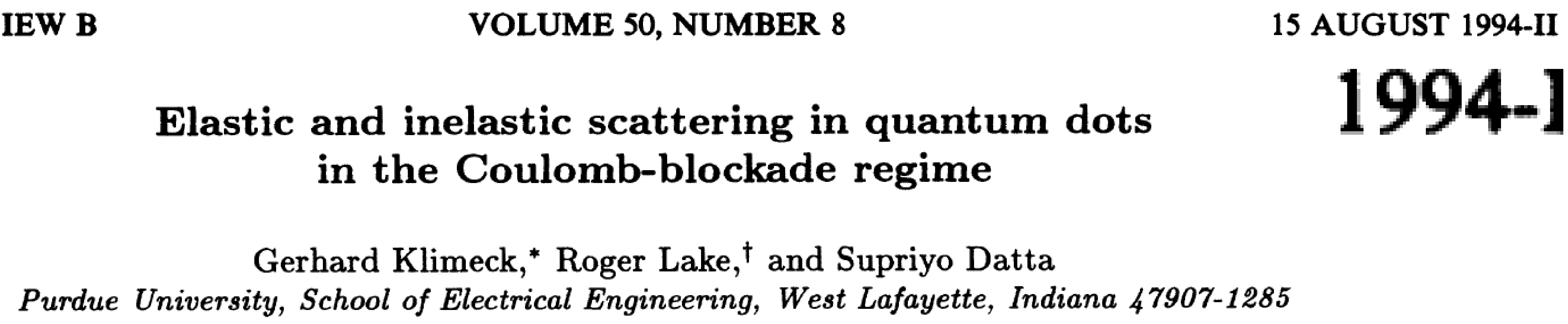




Choose the most probable configuration.

Occupation Statistics




PHYSICAL REVIEW B VOLUME 50, NUMBER 8 15 AUGUST 1994-II

1994-]

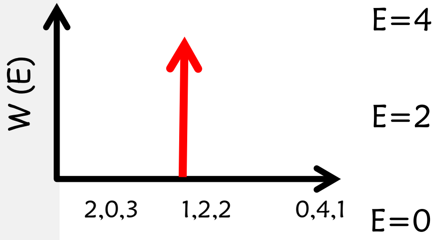
Elastic and inelastic scattering in quantum dots in the Coulomb-blockade regime

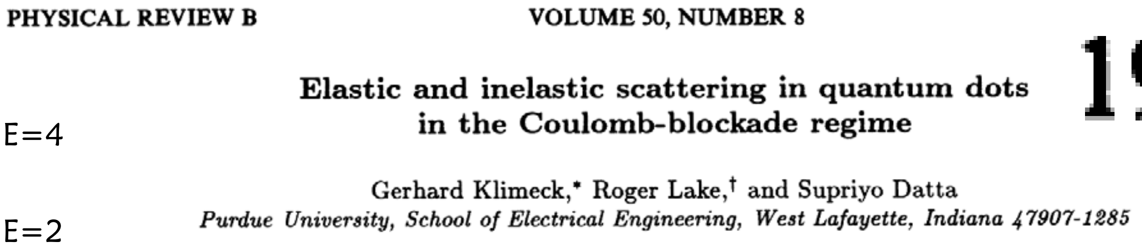
Gerhard Klimeck,* Roger Lake,† and Supriyo Datta
Purdue University, School of Electrical Engineering, West Lafayette, Indiana 47907-1285

Side note:
So far everything shown here is EXACT!
No approximations on the occupation probability!
=> direct application to nano-scale electronics!

Coulomb blockage
Single electronics

Occupation Statistics

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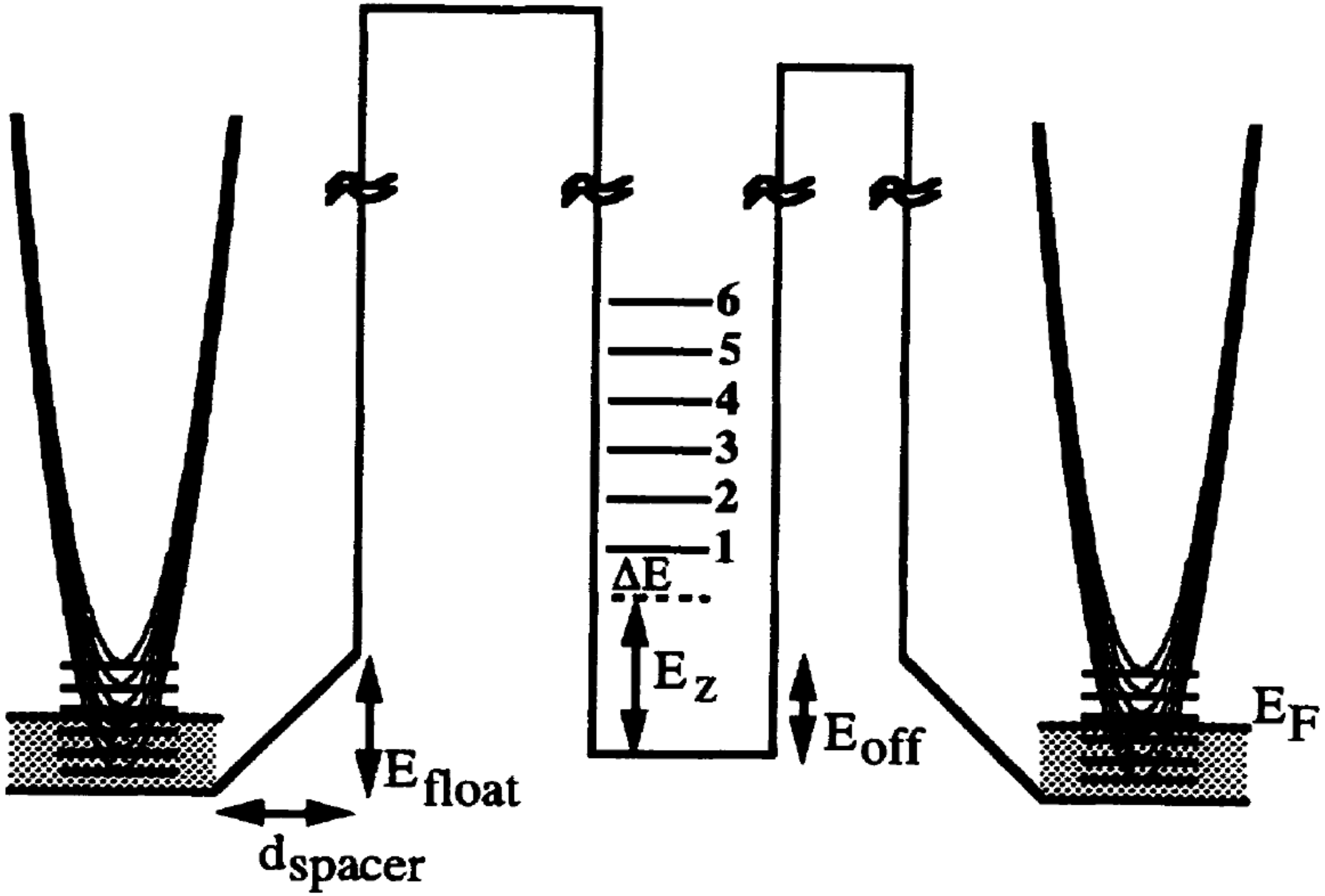

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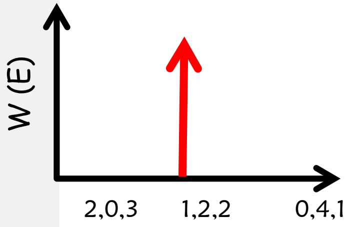

E=4

E=2

E=0

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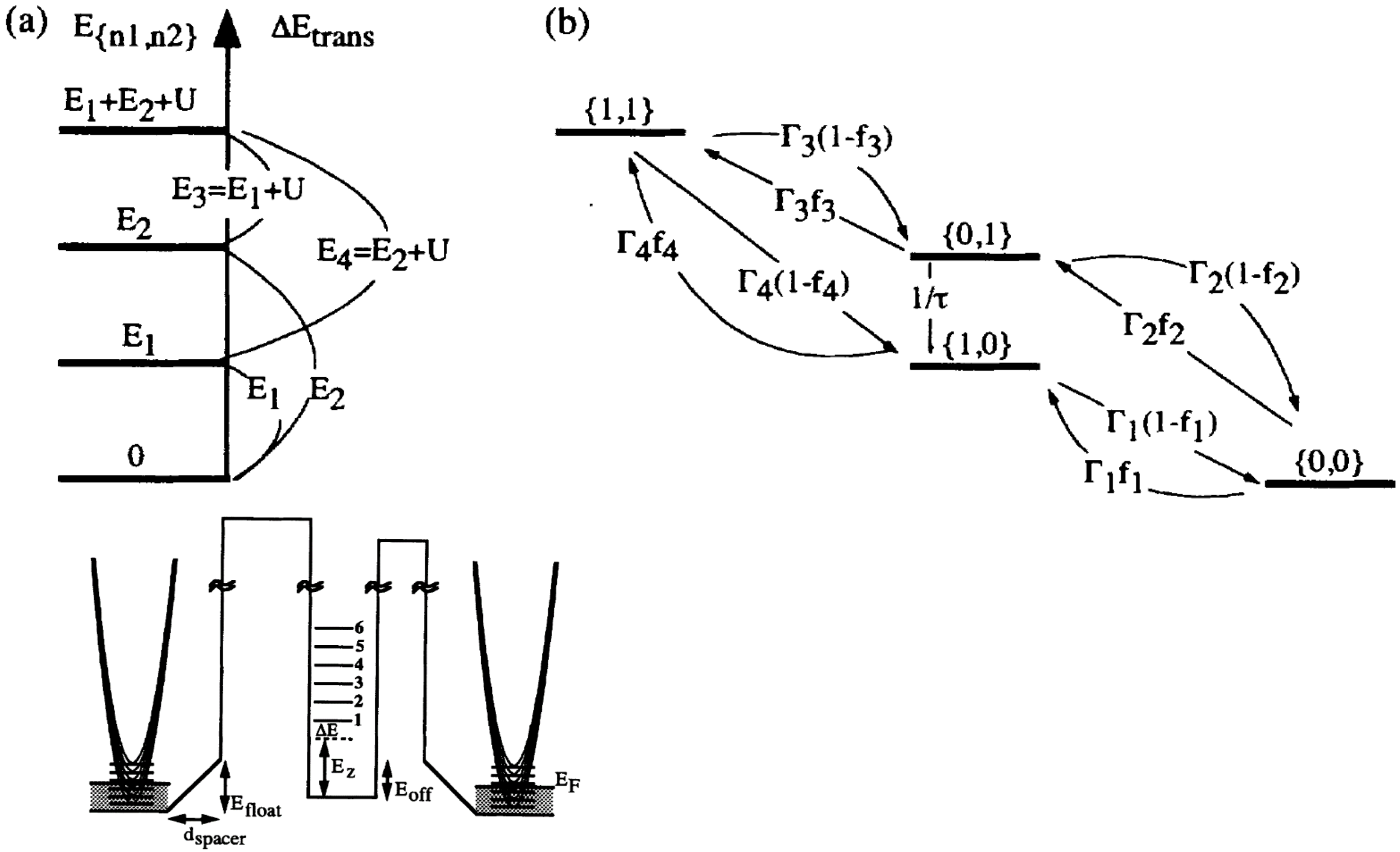

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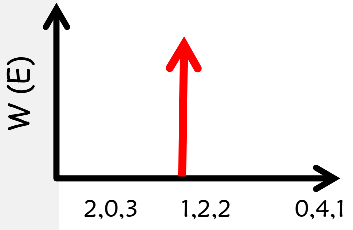

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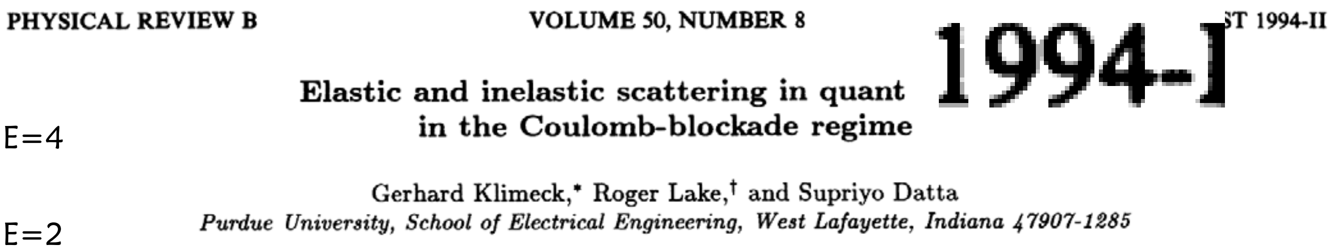
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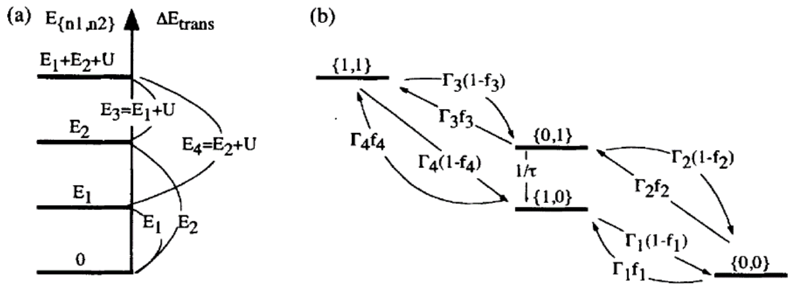

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Coulomb blockage
Single electronics

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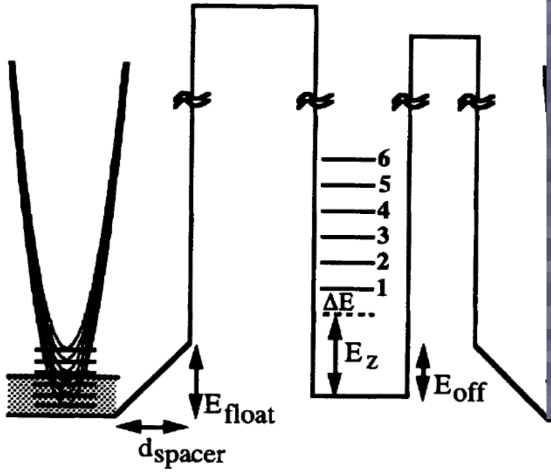
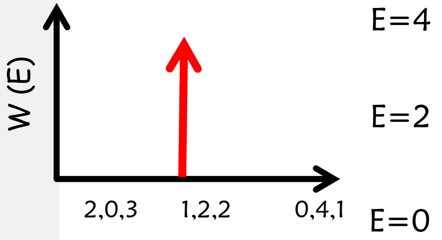
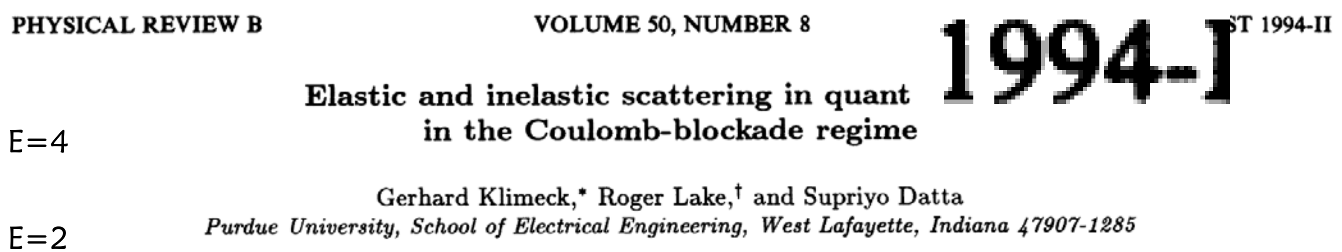


Occupation Statistics





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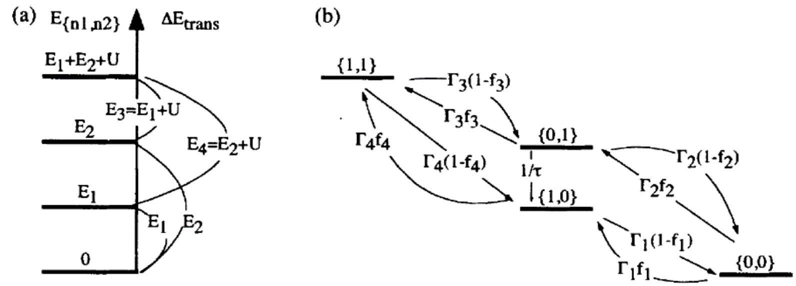

nature nanotechnology

PUBLISHED ONLINE: 19 FEBRUARY 2012 |

A single-atom transistor

Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapatra[1], Hoon Ryu[2], Sunhee Lee[3], Oliver Warschkow[4], Lloyd C. L. Hollenberg[5], Gerhard Klimeck[3] and Michelle Y. Simmons[1]*

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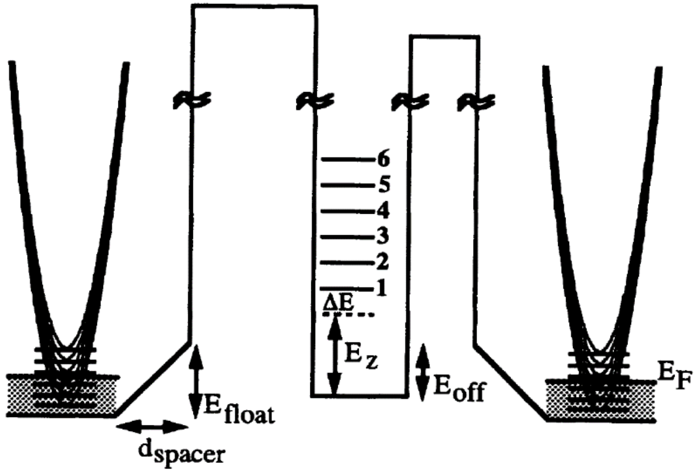
Coulomb blockage
Single electronics



Occupation Statistics

E=4

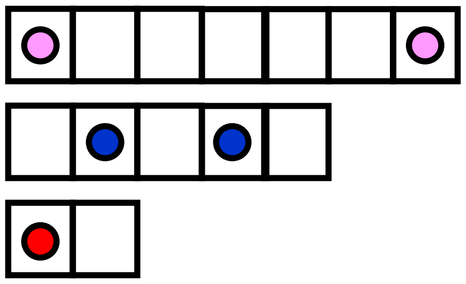
E=2

E=0

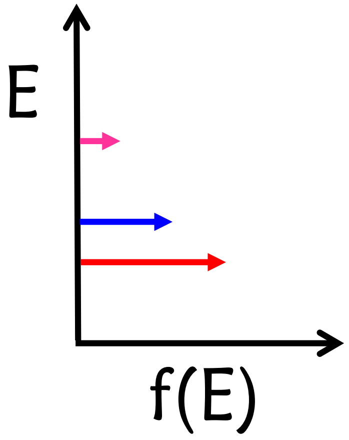
$$f_3^* = \frac{2}{7}$$

$$f_2^* = \frac{2}{5}$$

$$f_1^* = \frac{1}{2}$$



$$W_{122} = 420$$



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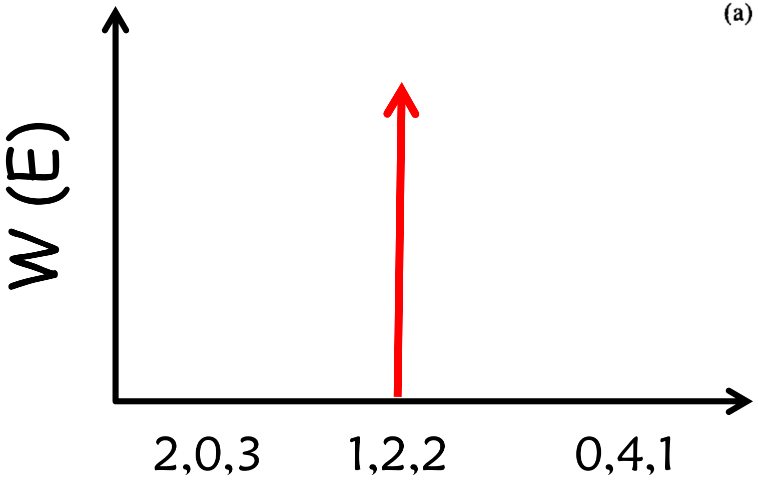

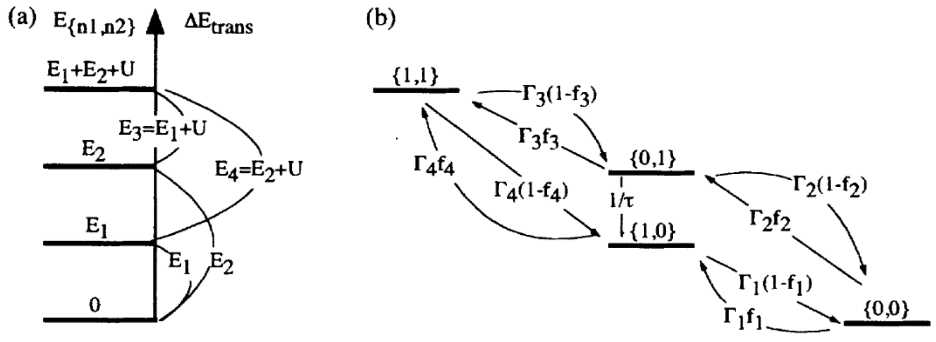

Coulomb blockage
Single electronics

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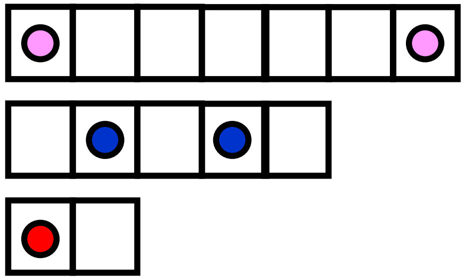

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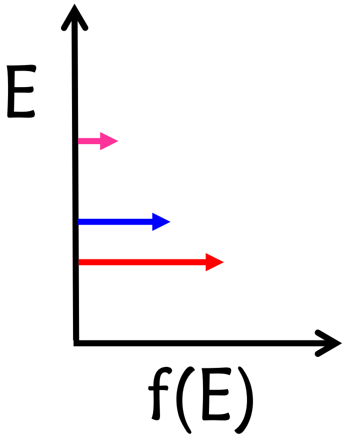
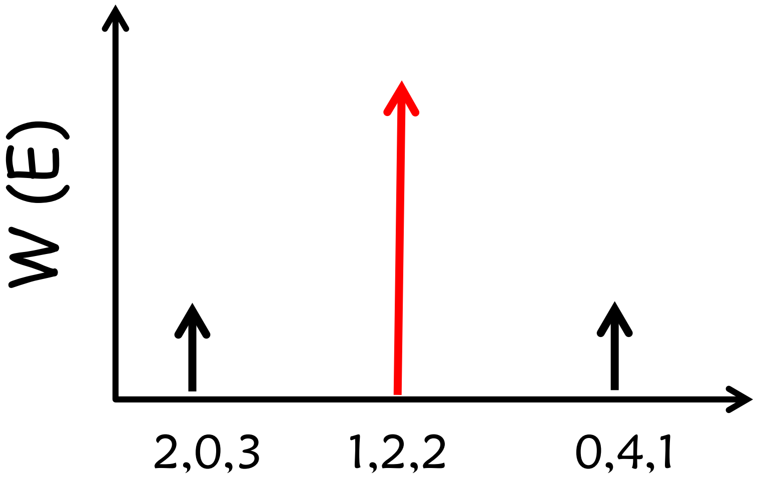
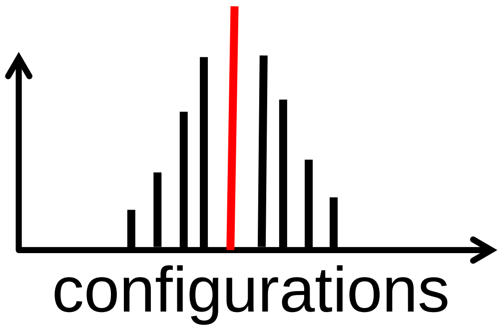


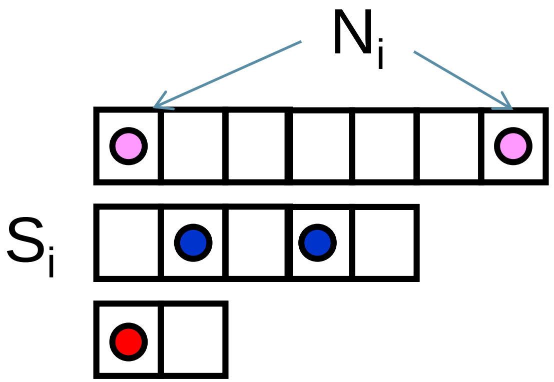


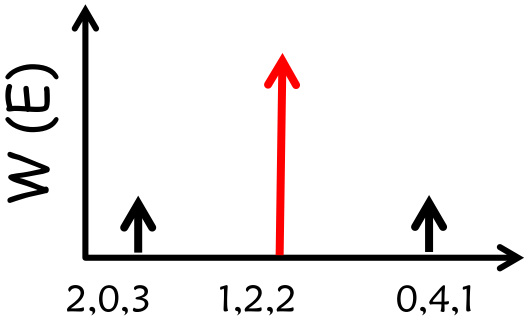


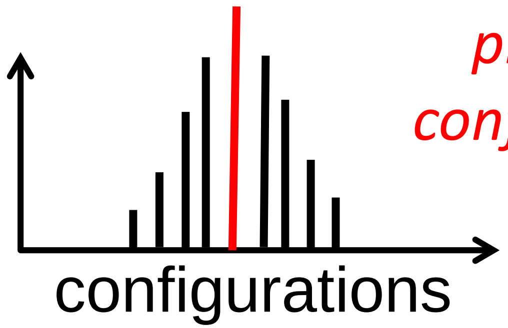
~~Coulomb blockage~~
~~Single electronics~~

For large numbers of states, what is the most probably configuration?

Occupation Statistics







Choose the most probable configuration.

$$W_c = \prod_i \frac{S_i!}{(S_i - N_i)!N_i!}$$

Recall. $W_{203} = \frac{2!}{1!2!} \bullet \frac{5!}{0!5!} \bullet \frac{7!}{3!4!}$

Stirling approx.

$$\ln(S!) \approx S\ln(S) - S \quad for \quad S > 10$$

$$\ln(W) = \sum_i [\ln S_i! - \ln(S_i - N_i)! - \ln N_i!]$$

$$\approx \sum_i [S_i \ln S_i - S_i - (S_i - N_i)\ln(S_i - N_i) + (S_i - N_i) - N_i \ln N_i + N_i]$$

$$\ln W = \sum_i [S_i \ln S_i - (S_i - N_i)\ln(S_i - N_i) - N_i \ln N_i]$$

For large numbers of states, what is the most probably configuration?

Optimization with Lagrange-Multiplier

$$\ln W = \sum_i \left[S_i \ln S_i - (S_i - N_i)\ln(S_i - N_i) - N_i \ln N_i \right]$$

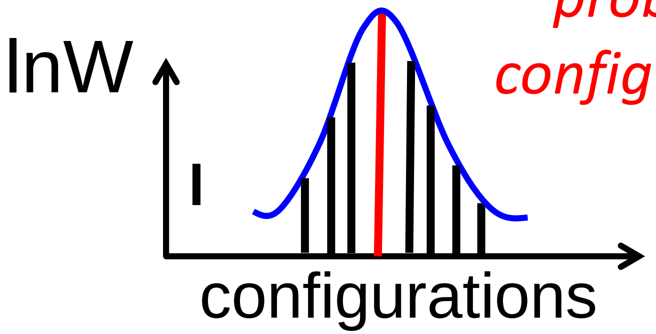
$$\delta \ln(W) = \sum_i \frac{\partial \ln W}{\partial N_i} dN_i$$

$$= \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) dN_i \right]$$

$$\square \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) dN_i \right] - \alpha \sum_i dN_i - \beta \sum_i E_i dN_i$$

$$= \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] dN_i$$

$$\delta \ln W = \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1 \right) - \alpha - \beta E_i \right] dN_i = 0$$



Choose the most probable configuration.

Optimization with constraints!

Energy conservation

$$E_T = \sum_i E_i N_i$$

Particle conservation

$$N_T = \sum_i N_i$$

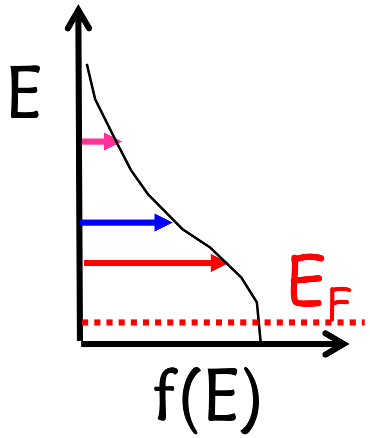
Lagrange multipliers at https://en.wikipedia.org/wiki/Lagrange_multiplier

For large numbers of states, what is the most probably configuration?

Final steps ...

$$\delta \ln W = \sum_i \left[\ln\left(\frac{S_i}{N_i} - 1\right) - \alpha - \beta E_i \right] dN_i = 0$$

$$\left[\ln\left(\frac{S_i}{N_i} - 1\right) - \alpha - \beta E_i \right] = 0$$



$$f(E) \equiv \frac{N_i}{S_i} = \frac{1}{1+e^{\alpha+\beta E}}$$

$f_{\text{max}}(\text{E})=1$

At $E = E_F, \quad f(E_F) \equiv \frac{1}{2} \quad \Rightarrow \alpha + \beta E_F = 0$

$$f(E) = \frac{N_i}{S_i} = \frac{1}{1+e^{\beta(E-E_F)}} = \frac{1}{1+e^{(E-E_F)/k_B T}}$$

$$f_0(E) = \frac{1}{1+e^{\beta(E-E_F)}}$$

At $E \to \infty, \quad f_{Boltzman}(E) = Ae^{-E/k_B T} \quad \Rightarrow \quad \beta = \frac{1}{k_B T}$

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One Video Segment

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  - Pauli exclusion
  - Total particle conservation
  - Total energy conservation

Carrier number =
Number of states x ***filling factor***

$$f_0(E) = \frac{1}{1+e^{\beta(E-E_F)}}$$

One Video Segment

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  - Microcanonical ensemble - statistics
  - Detailed Balance – thermal equilibrium & Pauli exclusion
  - Partition Function – statistical mechanics

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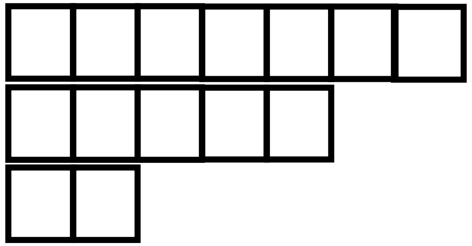
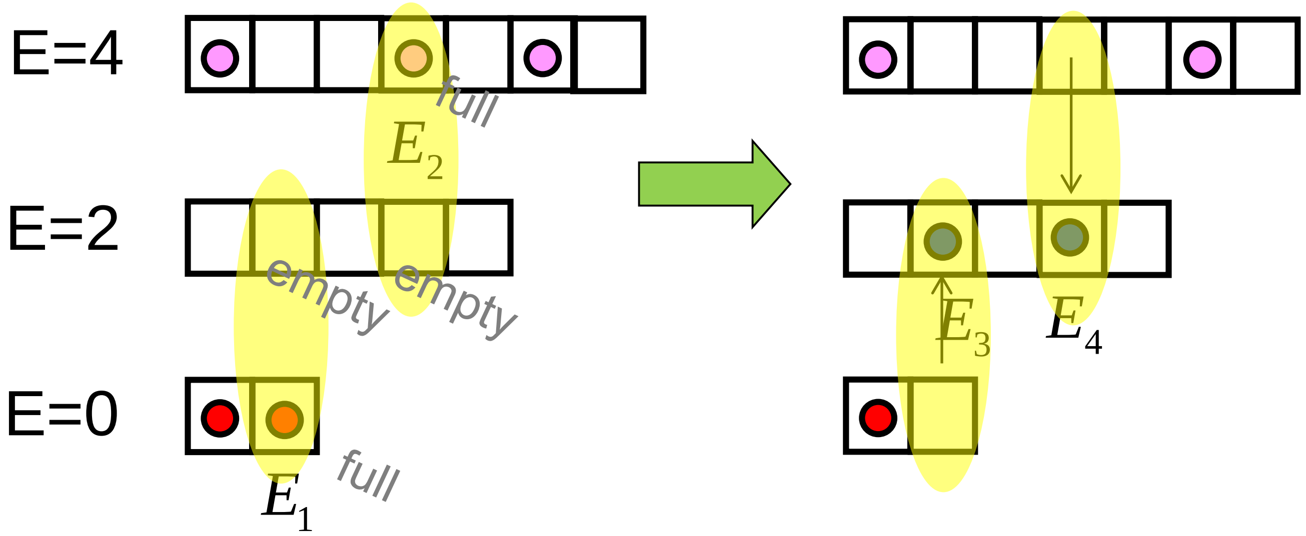


One Video Segment

- 12.3 Intrinsic carrier concentration

Reference: Vol. 6, Ch. 4

Derivation by Detailed Balance



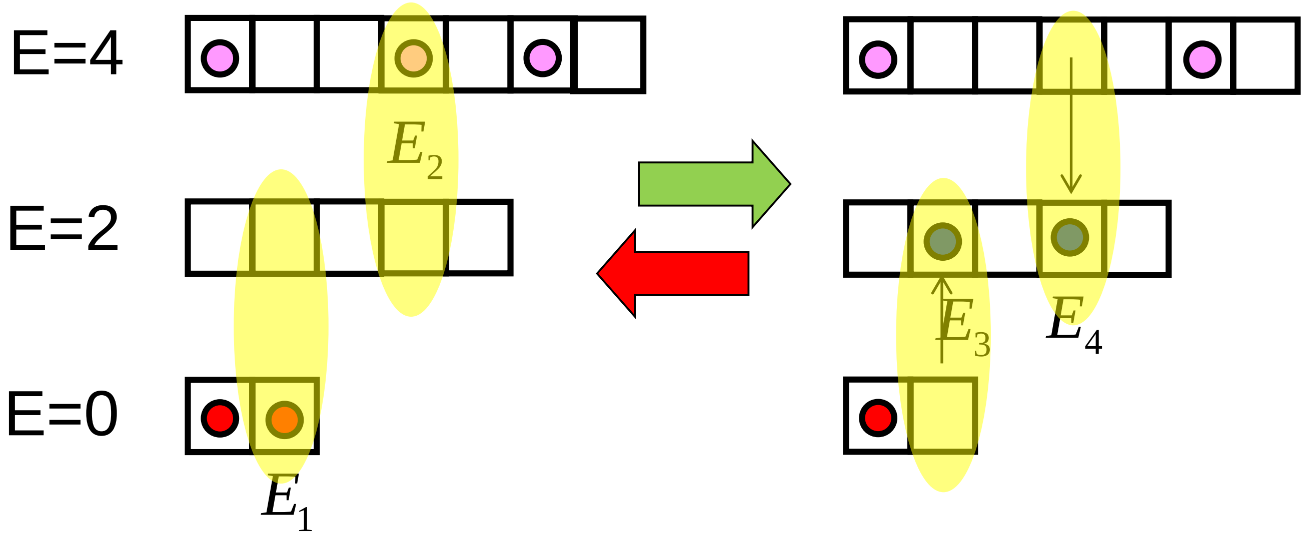
Detailed Balance in Equilibrium

full full empty empty

$$f_0(E_1)\,f_0(E_2)[1-f_0(E_3)][1-f_0(E_4)]$$

➡ Pauli Exclusion

Derivation by Detailed Balance



Detailed Balance in Equilibrium

$$f_0(E_1)\,f_0(E_2)[1-f_0(E_3)][1-f_0(E_4)]$$

Pauli Exclusion

$$= f_0(E_3)\,f_0(E_4)[1-f_0(E_1)][1-f_0(E_2)]$$

Energy conversation

$$E_1 + E_2 = E_3 + E_4$$

Only solution is ….
$$f_0(E) = \frac{1}{1+e^{\beta(E-E_F)}}$$

- Pauli Principle, energy, and number conservation all satisfied

A Note on the Use of the Principle of Detailed Balance in Obtaining the Fermi-Dirac Distribution Function, John E. Walsh: American Journal of Physics38, 392 (1970); doi: 10.1119/1.1976344

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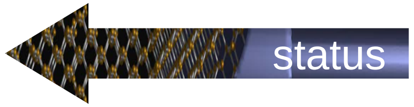
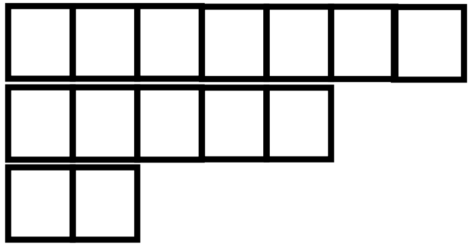


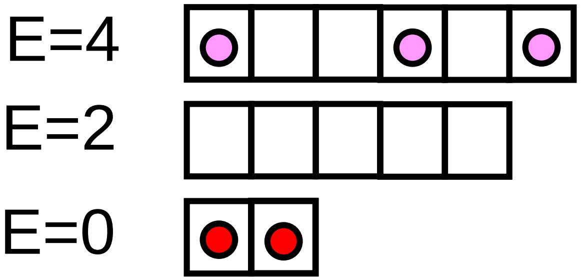


One Video Segment

- 12.3 Intrinsic carrier concentration

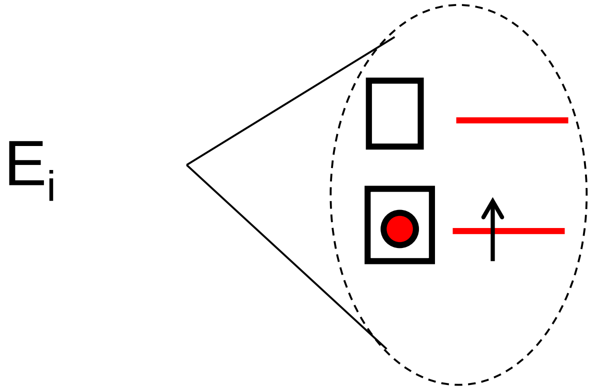
Reference: Vol. 6, Ch. 4

Derivation by Partition Function



$$P_i = \frac{e^{-\beta(E_i - N_i E_F)}}{\sum_i e^{-\beta(E_i - N_i E_F)}} \equiv \frac{e^{-\beta(E_i - N_i E_F)}}{Z}$$

$$\beta = 1/k_B T$$



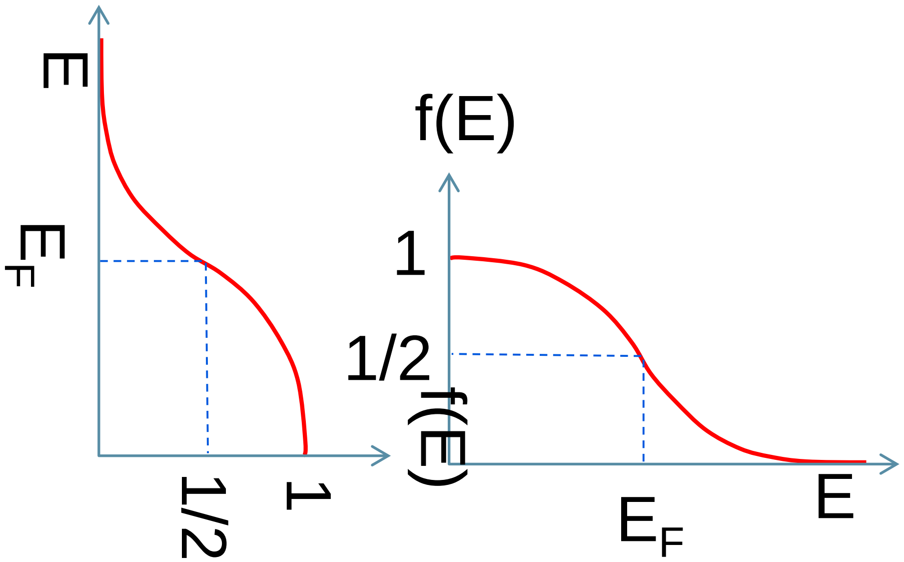
state	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

Derivation by Partition Function

1

$state$	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

Probability that state is filled ….



$$f(E)=\frac{P_1}{P_0+P_1}$$

$$=\frac{e^{-(E_i-E_F)/k_BT}\;/\;Z}{1/Z+e^{-(E_i-E_F)/k_BT}\;/\;Z}$$

$$=\frac{1}{1+e^{(E_i-E_F)/k_BT}}$$

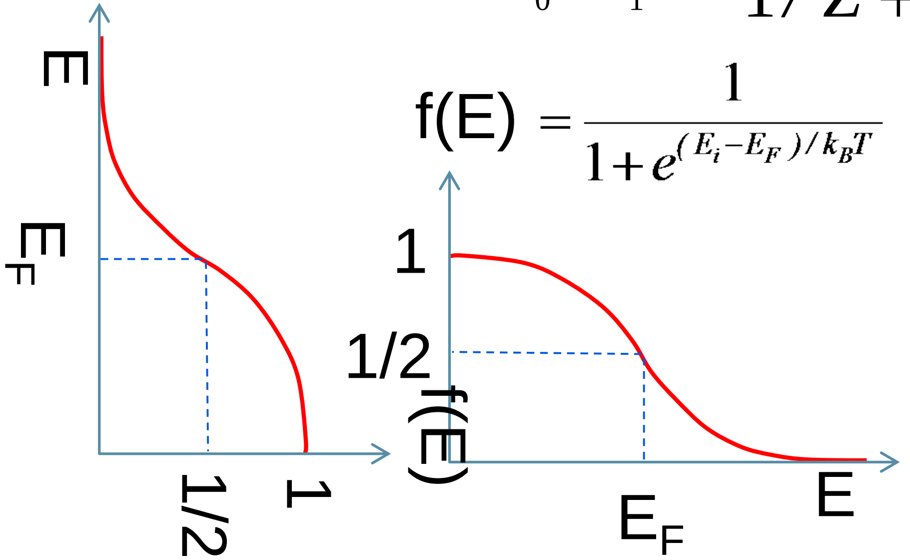
Derivation by Partition Function

1

state	E_i	N_i	P_i
0	0	0	$e^{-\beta(0-0\times E_F)}/Z$
1	1	1	$e^{-\beta(E_i-1\times E_F)}/Z$

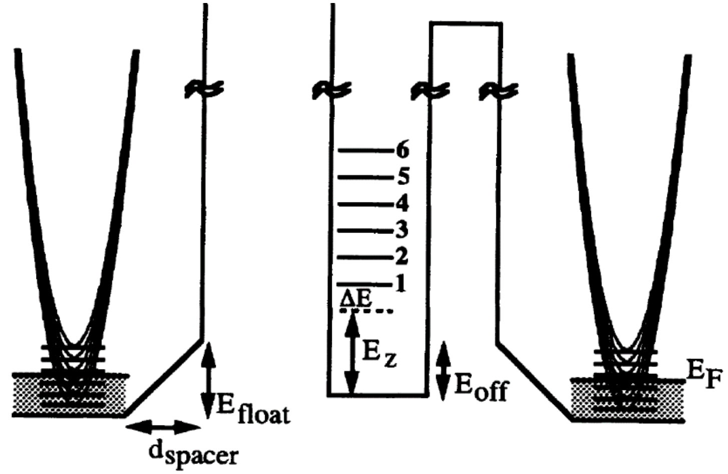
Probability that state is filled ….

$$f(E)=\frac{P_1}{P_0+P_1}=\frac{e^{-(E_i-E_F)/k_BT}\ /\ Z}{1/Z+e^{-(E_i-E_F)/k_BT}\ /\ Z}$$



$$\text{f(E)}=\frac{1}{1+e^{(E_i-E_F)/k_BT}}$$

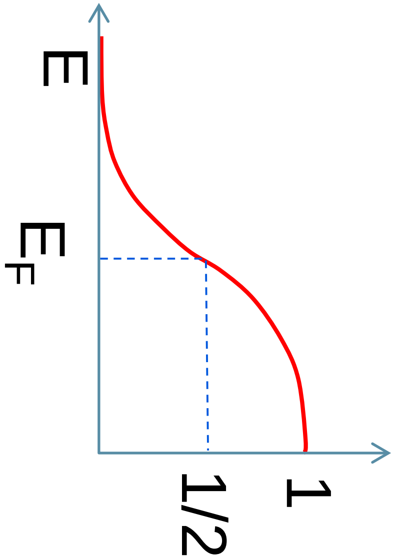
Elastic and inelastic scattering in quantum dots in the Coulomb-blockade regime



$$P_0(\{m_k\})=\frac{\mathcal{D}(\{m_k\})\ \exp\left(\sum_{p=1}^{\infty}E_pm_p\Big/k_BT\right)}{\sum_{\{o_k\}}\mathcal{D}(\{o_k\})\ \exp\left(\sum_{p=1}^{\infty}E_po_p\Big/k_BT\right)\ \delta_{N,\sum_p o_p}}\,P(N)\ .$$

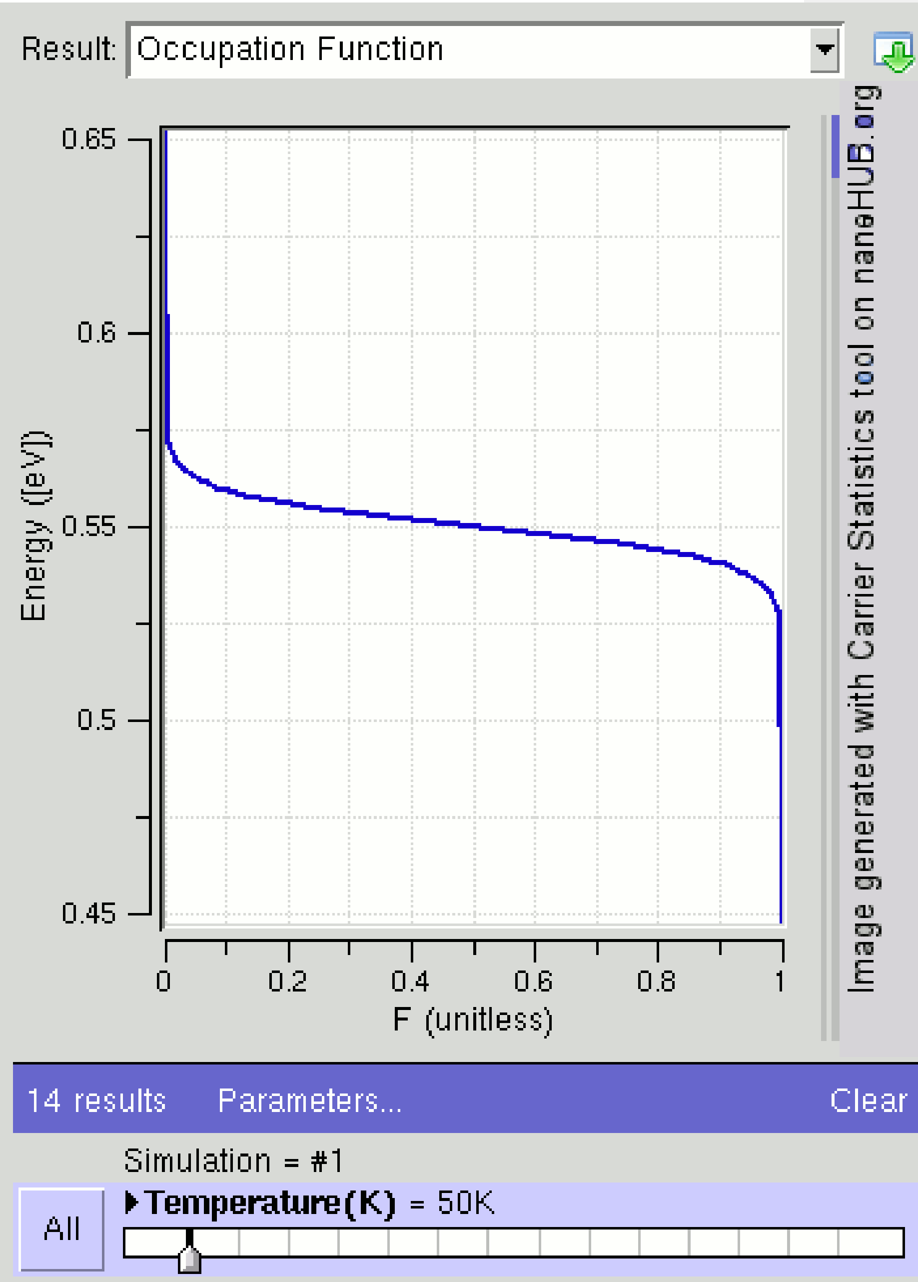
Partition Function or Statistical Mechanics Approach also holds for single electronics!

Temperature Dependence



$$f(E) = \frac{1}{1+e^{(E_i - E_F)/k_B T}}$$

Hot electrons reach higher energy states
Cold electrons are “frozen” to lowest possible states


Result: Occupation Function

Simulation = #1

Temperature(K) = 50K

https://commons.wikimedia.org/wiki/File:Fermi.gif
another nanoHUB animation on Wikipedia
https://nanohub.org/tools/fermi

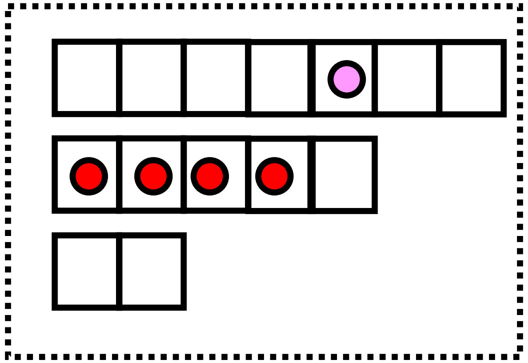
Few comments on Fermi-Dirac Statistics

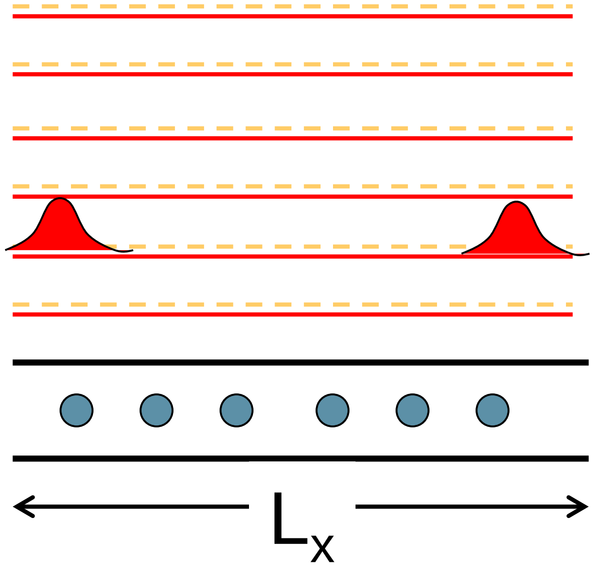
- Applies to all spin-1/2 particles

- Typically, information about spin is not explicit; multiply DOS by 2.
  May be more complicated for magnetic semiconductors,
  Topological insulators, quantum computing, coulomb blockade etc

- Coulomb-interaction among particles is neglected,
  Therefore it applies to extended solids, not to small molecules

$$\frac{1}{1+e^{(E_i-E_F)/k_BT}}$$





Section 12
Occupation of States

One Video Segment

- 12.1 Rules of filling electronic states
  - » Pauli exclusion
  - » Total particle conservation
  - » Total energy conservation

Carrier number =
Number of states x ***filling factor***

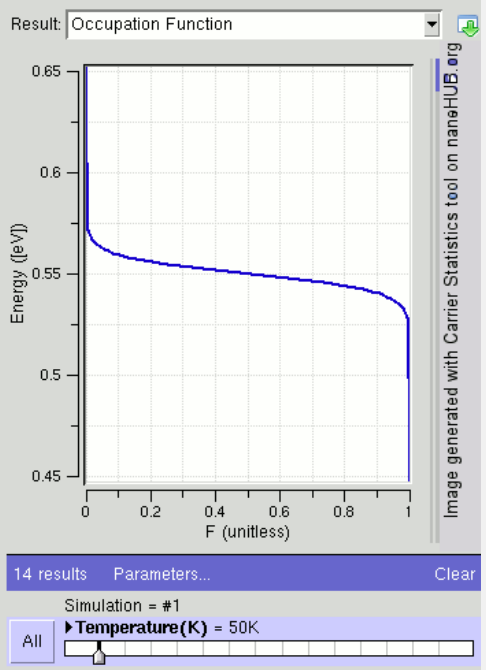
$$\frac{1}{1+e^{(E_i-E_F)/k_BT}}$$

One Video Segment

- 12.2 Derivation of Fermi-Dirac Statistics: three techniques
  - » Microcanonical ensemble - statistics
  - » Detailed Balance – thermal equilibrium & Pauli exclusion
  - » Partition Function – statistical mechanics

status

In 1926, Fowler studied collapse of a star to white dwarf by F-D statistics, before Sommerfeld used the F-D statistics to develop a theory of electrons in metals in 1927. Wikipedia has a nice article on this topic.



Simulation = #1
Temperature(K) = 50K

One Video Segment

- 12.3 Intrinsic carrier concentration

Reference: Vol. 6, Ch. 4

Section 12
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One Video Segment

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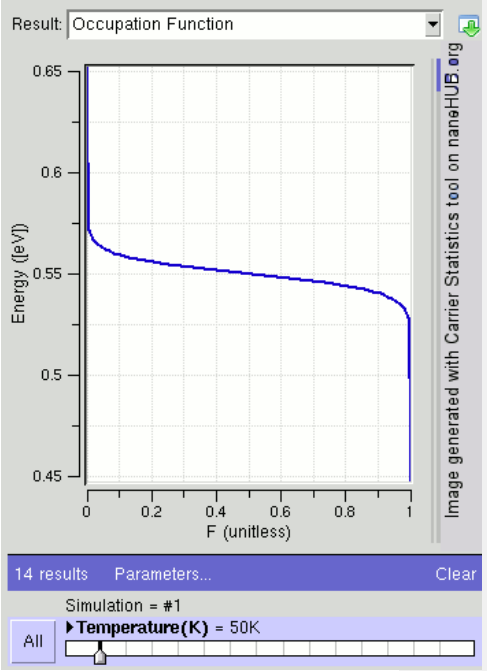


Result: Occupation Function

Simulation = #1

Temperature(K) = 50K

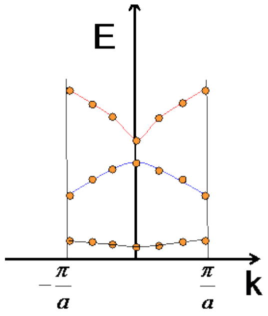
One Video Segment

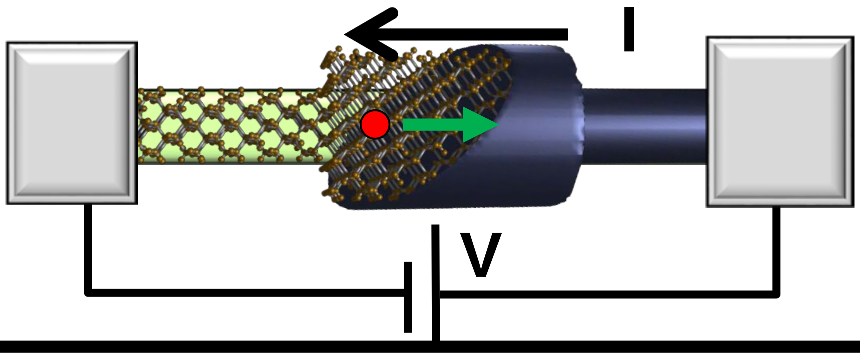
- 12.3 Intrinsic carrier concentration
  - Fermi Integral
  - Law of mass action

status

Reference: Vol. 6, Ch. 4

Section 12
Occupation of States





$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area

- **Materials, composition, crystals**
- Tabulated for “known” bulk materials
- ~~[illegible] properties [illegible] with geometry [illegible] theory~~

~~⇒ **Quantum Mechanics Mechanics**~~
- Concepts of density of states and masses

⇒ **Equilibrium Statistical Mechanics**
- Occupation factors

$$f_0(E) = \frac{1}{1+e^{\beta(E-E_F)}} \qquad N_C \equiv 2\left(\frac{2\pi m_n^* \beta}{h^2}\right)^{3/2}$$

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c) \rightarrow N_C e^{-\beta(E_c - E_F)}$$

$$E_i = \frac{E_G}{2} + \frac{1}{2\beta} ln \frac{N_V}{N_C} \qquad n \times p = N_C N_V e^{-\beta(E_c - E_v)}$$
$$= N_C N_V e^{-\beta E_g}$$

Transport with scattering, non-equilibrium Statistical Mechanics
- Drift-diffusion equation with recombination-generation

Understanding transport in concrete devices
- Diodes, BJT/HBT, MOS