ECE 659 Quantum Transport: Atom to Transistor

Lecture 39: Singlet/Triplet States II

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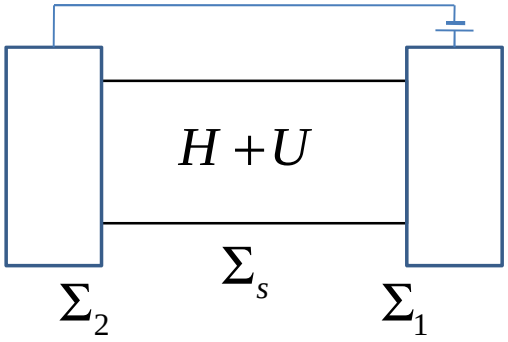
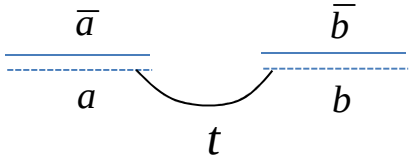




No. of Electrons	Size of Hamiltonian
0	1x1
1	4x4
2	6x4
3	4x4
4	1x1

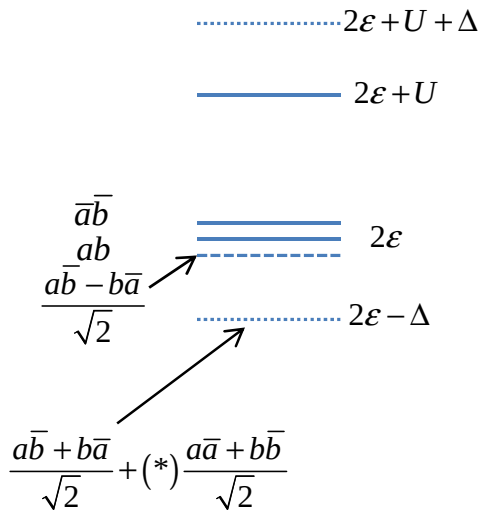
1&3 electron subspace:

$$H = \begin{array}{c} \\ a \\ b \\ \bar{a} \\ \bar{b} \end{array} \begin{array}{c} \begin{array}{cccc} a & b & \bar{a} & \bar{b} \end{array} \\ \begin{bmatrix} \varepsilon & t & & \\ t & \varepsilon & & \\ & & \varepsilon & t \\ & & t & \varepsilon \end{bmatrix} \end{array}$$

2 electron subspace:

	$a\bar{a}$	$b\bar{b}$	$a\bar{b}$	$b\bar{a}$	ab	$\bar{a}\bar{b}$
$a\bar{a}$	$2\varepsilon+U$		t	t		
$b\bar{b}$		$2\varepsilon+U$	t	t		
$a\bar{b}$	t	t	2ε			
$b\bar{a}$	t	t		2ε		
ab					2ε	
$\bar{a}\bar{b}$						2ε

For 2 electrons the eigen energies are:



Lowest energy states:

Molecular Orbital Theory:

$$\frac{1}{2}(a+b)\otimes(\bar{a}+\bar{b})=\frac{1}{2}(a\bar{a}+b\bar{b}+b\bar{a}+a\bar{b})$$

We see from the multi-electron picture that $a\bar{a}$ and $b\bar{b}$ terms get de-emphasized, which is not clear from MO theory. If 't' is large, we can work with MO theory and factorize the wavefunction. If 't' is small this is not possible.

In general we can us 'Schrodinger Eqn.' for the complete system:

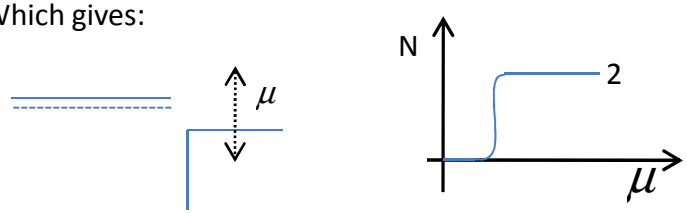
$$i\hbar\frac{\partial\bar{\psi}}{\partial t}=\bar{H}\bar{\psi}$$

$\bar{H}$ is the Hamiltonian for the complete system

Now,

$$P_i=\frac{1}{Z}e^{-(E_i-\mu N_i)/k_BT}$$

Which gives:

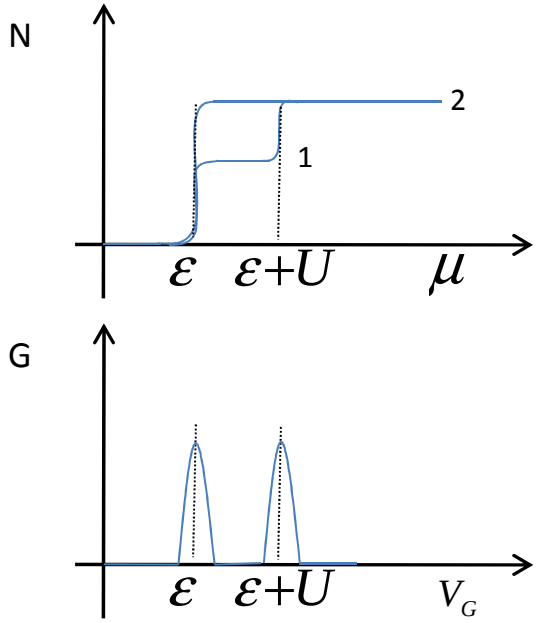


in case of no interaction

In case of non-zero interaction energy:

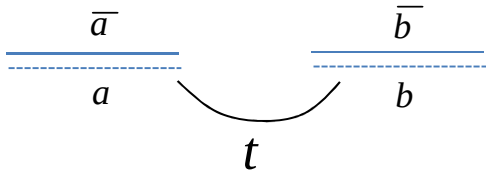
	$E_i - \mu N_i$
11	$2\varepsilon+U$ $\quad$ $2\varepsilon+U-2\mu$
01 $\quad$ 10	ε $\quad$ $\varepsilon-\mu$
00	0 $\quad$ 0

$P_i = 1$ for system with minimum $E_i - \mu N_i$

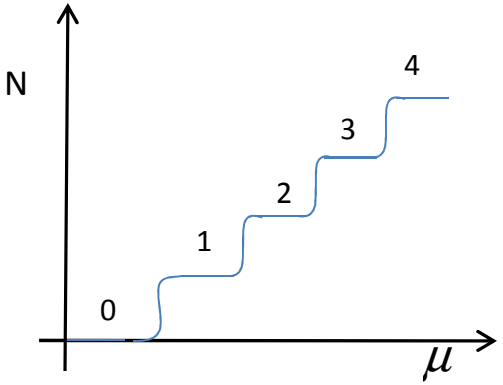


$E_i - \mu N_i$	P_i	
100	$e^{-100}/e^{-100}+e^{-200}$	$\to 1$
200	$e^{-200}/e^{-100}+e^{-200}$	$\to 0$

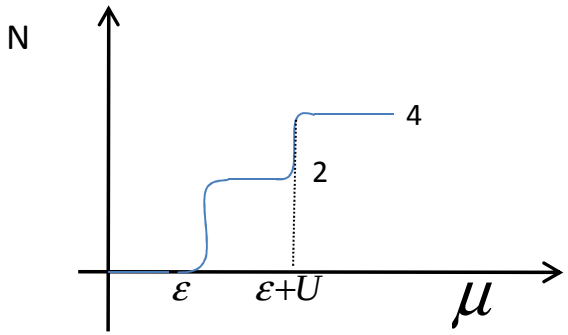
Double Quantum Dots



$$P_i = \frac{1}{Z} e^{-(E_i - \mu N_i)/k_B T}, \langle N \rangle = \sum_i P_i N_i$$



With t =0 and same U on both the dots we get:



With non-zero t and same U on both dots we get as before

$$P_i = \frac{1}{Z} e^{-(E_i - \mu N_i)/k_B T}$$

A more general version is:

$$\rho = \frac{1}{Z} \exp\left[-\frac{H - \mu N}{k_B T} \right]$$

$$\langle N \rangle = \sum_i \rho_{ii} N_{ii} = Trace(N\rho)$$