

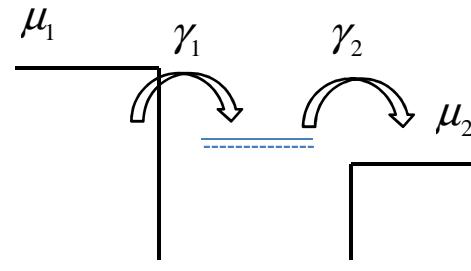
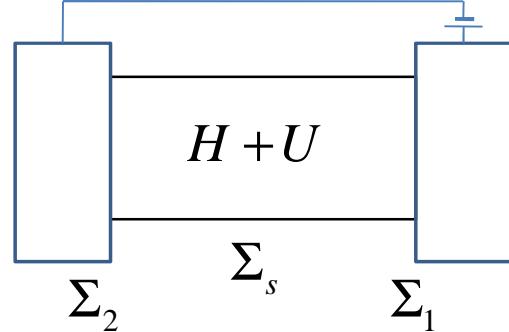
ECE 659 Quantum Transport: Atom to Transistor

Lecture 38: Singlet/Triplet States

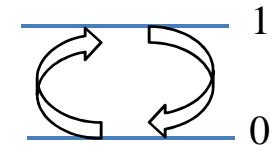
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Notes prepared by Samiran Ganguly

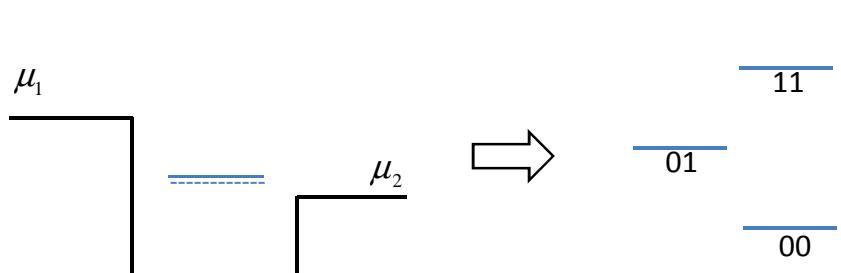
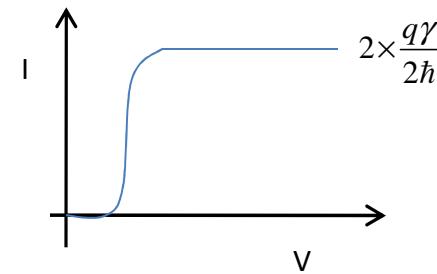


One electron picture



Multi-electron picture

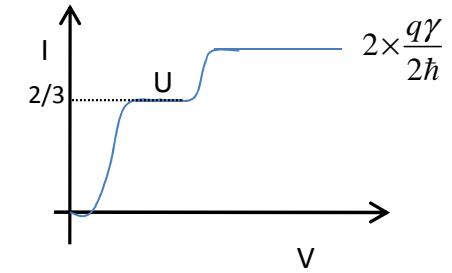
N electrons $\rightarrow 2^N$ states in multi-electron picture



$2\epsilon + U$

ϵ

0



Hydrogen Molecule/Quantum Dots :



Hamiltonian for 2 separate atoms/dots:

$$H = \begin{matrix} a & b \\ b & \epsilon \end{matrix} \quad \begin{matrix} \epsilon - t \\ \epsilon + t \end{matrix}$$

$$\frac{a+b}{\sqrt{2}}$$

Hamiltonian with the down-spin level*:

$$H = \begin{matrix} a & b & \bar{a} & \bar{b} \\ b & \epsilon & t & \\ \bar{a} & t & \epsilon & \\ \bar{b} & & t & \epsilon \end{matrix}$$

*empty spots in the matrices will mean 0 now onwards

In total we have $16(2^4)$ states

$$\{0000\} \rightarrow 1$$

$$\{0001\} \rightarrow 4$$

$$\{0011\} \rightarrow 6$$

$$\{0111\} \rightarrow 4$$

$$\{1111\} \rightarrow 1$$

We shall concentrate on the 2-electron problem

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

$a\bar{a} \rightarrow b\bar{b}$ includes a spin flip process, we are considering only tunneling processes here, so we put 0

Eigen Values:

Obvious ones: 2ϵ

$$\begin{array}{c} \overline{ab} \\ \overline{ab} \end{array}$$

To solve rest of the Hamiltonian analytically, we define following linear combinations:

$$a\bar{a} \begin{bmatrix} B & A \\ b\bar{b} & 1 \end{bmatrix} \frac{1}{\sqrt{2}} \quad a\bar{b} \begin{bmatrix} S & T \\ b\bar{a} & 1 \end{bmatrix} \frac{1}{\sqrt{2}}$$

We get*:

$$\begin{bmatrix} B & A & S & T \\ 2\epsilon + U & 2t & 2\epsilon & 2\epsilon \\ A & 2\epsilon + U & & \\ S & 2t & 2\epsilon & \\ T & & & 2\epsilon \end{bmatrix}$$

$$* \quad \frac{1}{2} B \begin{bmatrix} a\bar{a} & b\bar{b} \\ 1 & 1 \end{bmatrix} a\bar{a} \begin{bmatrix} ab & b\bar{a} \\ t & t \end{bmatrix} a\bar{b} \begin{bmatrix} S & T \\ b\bar{a} & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2t \\ \end{bmatrix}$$

$$\begin{array}{ccccc} A & B & S & T \\ 2\epsilon + U & & & \\ & 2\epsilon + U & 2t & \\ & 2t & 2\epsilon & \\ & & & 2\epsilon \end{array}$$

