ECE 659 Quantum Transport: Atom to Transistor

Lecture 28: Spin Orbit Interaction II

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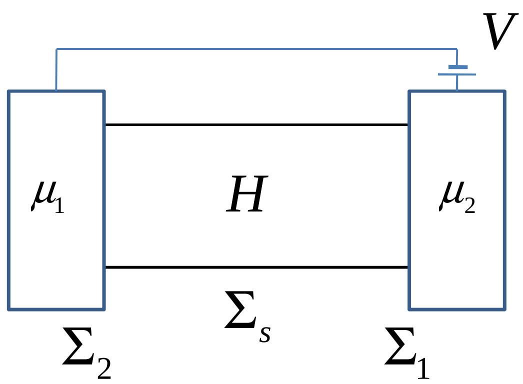
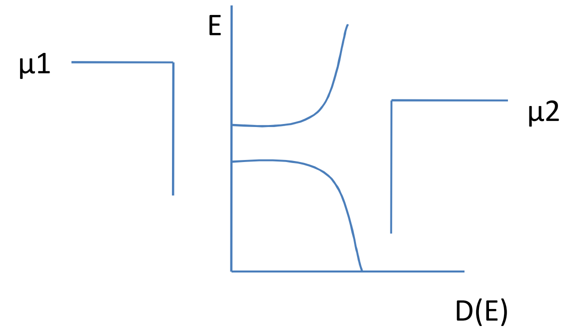




Schrodinger Equation:

1x1 differential equation

$$\left(i\hbar\frac{\partial}{\partial t}+qV\right)\psi=\frac{\left(\vec{p}+q\vec{A}\right)\cdot\left(\vec{p}+q\vec{A}\right)}{2m}\psi$$

$$\vec{p}=-i\hbar\nabla$$

$$\vec{B}=\nabla\times\vec{A}$$

$$\vec{E}=-\nabla V-\frac{\partial\vec{A}}{\partial t}$$

Dirac Equation:

4x4 differential equation

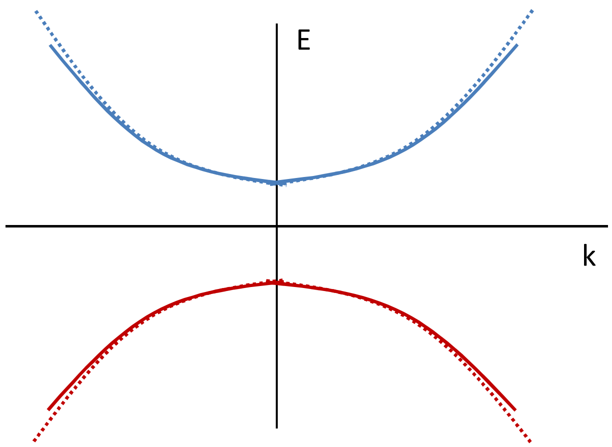
$$\left(i\hbar\frac{\partial}{\partial t}+qV\right)\begin{Bmatrix}\psi\\ \phi\end{Bmatrix}=\begin{bmatrix} mc^2 I & c\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right)\\ c\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right) & -mc^2 I\end{bmatrix}\begin{Bmatrix}\psi\\ \phi\end{Bmatrix}$$

ψ,ϕ,σ,p are all 2x2 matrix, I is a 2x2 identity matrix

$$\vec{\sigma}.\vec{p}=\begin{bmatrix} p_z & p_x-ip_y\\ p_x+ip_y & -p_z\end{bmatrix}$$

If V and A are 0, the solution is a plane wave: $e^{ikx}e^{-iEt/\hbar}$

E-k relation for Dirac Equation:



Pauli Equation:

2x2 differential equation

$$\left(i\hbar\frac{\partial}{\partial t}+qV\right)\psi=\frac{\left[\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right)\right]^2}{2m}\psi$$

$$\frac{c\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right)c\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right)}{E+mc^2}$$

$$\xrightarrow{E\sim mc^2}\frac{\left[\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right)\right]^2}{2m}$$

With a higher order approximation we get another term which is a relativistic correction term and is the spin-orbit coupling

$$\left(i\hbar\frac{\partial}{\partial t}+qV\right)\psi=\frac{\left[\vec{\sigma}\cdot\left(\vec{p}+q\vec{A}\right)\right]^2}{2m}\psi=\left(\frac{\left(\vec{p}+q\vec{A}\right)^2}{2m}I+\underbrace{\mu_B}_{\frac{q\hbar}{2m}}\vec{\sigma}\cdot\vec{B}\right)\psi$$

Now let: $\vec{A}=\nabla\chi(\vec{r},t)\quad\rightarrow\vec{B}=0$

$$V=-\frac{\partial\chi(\vec{r},t)}{\partial t}\quad\rightarrow\vec{E}=0$$

The Pauli equation has the above form due the requirement that if we put a V and A corresponding to the above special form of non zero potential the only change to the solution to Dirac Equation is:

$$\begin{Bmatrix}\psi\\\phi\end{Bmatrix}\rightarrow\begin{Bmatrix}\psi\\\phi\end{Bmatrix}e^{\chi q/i\hbar}$$

Original solution

Modified solution

This ensures that in case of 0 fields due to the special form of the potential the solution does not contain any unexpected results

Pauli Equation with relativistic correction:

$$\left(i\hbar\frac{\partial}{\partial t}+qV\right)\begin{Bmatrix}\psi\\ \bar{\psi}\end{Bmatrix}=\left(\frac{\left(\vec{p}+q\vec{A}\right)^2}{2m}I+\mu_B\vec{\sigma}\cdot\vec{B}+\mu_B\frac{\vec{\sigma}\cdot\left(\vec{E}\times\vec{p}\right)}{2mc^2}\right)\begin{Bmatrix}\psi\\ \bar{\psi}\end{Bmatrix}$$

$$\vec{\sigma}\cdot\left(\vec{E}\times\vec{p}\right)=\begin{bmatrix}E_x p_y-E_y p_x & \begin{matrix}E_y p_z-E_z p_y\\ -i\left(E_z p_y-E_y p_z\right)\end{matrix}\\ \begin{matrix}E_y p_z-E_z p_y\\ -i\left(E_z p_y-E_y p_z\right)\end{matrix} & E_y p_x-E_x p_y\end{bmatrix}$$

2 in vacuum

Rashba term

$$E\begin{Bmatrix}\psi\\ \bar{\psi}\end{Bmatrix}=\left(\frac{\left(\vec{p}+q\vec{A}\right)^2}{2m^*}I+\frac{g}{2}\underbrace{\mu_B}_{\frac{q\hbar}{2m}}\vec{\sigma}\cdot\vec{B}+\underline{\frac{\eta}{\hbar}\vec{\sigma}\cdot\left(\vec{z}\times\vec{p}\right)}\right)\begin{Bmatrix}\psi\\ \bar{\psi}\end{Bmatrix}$$

Free electron mass

Only for 2D structures