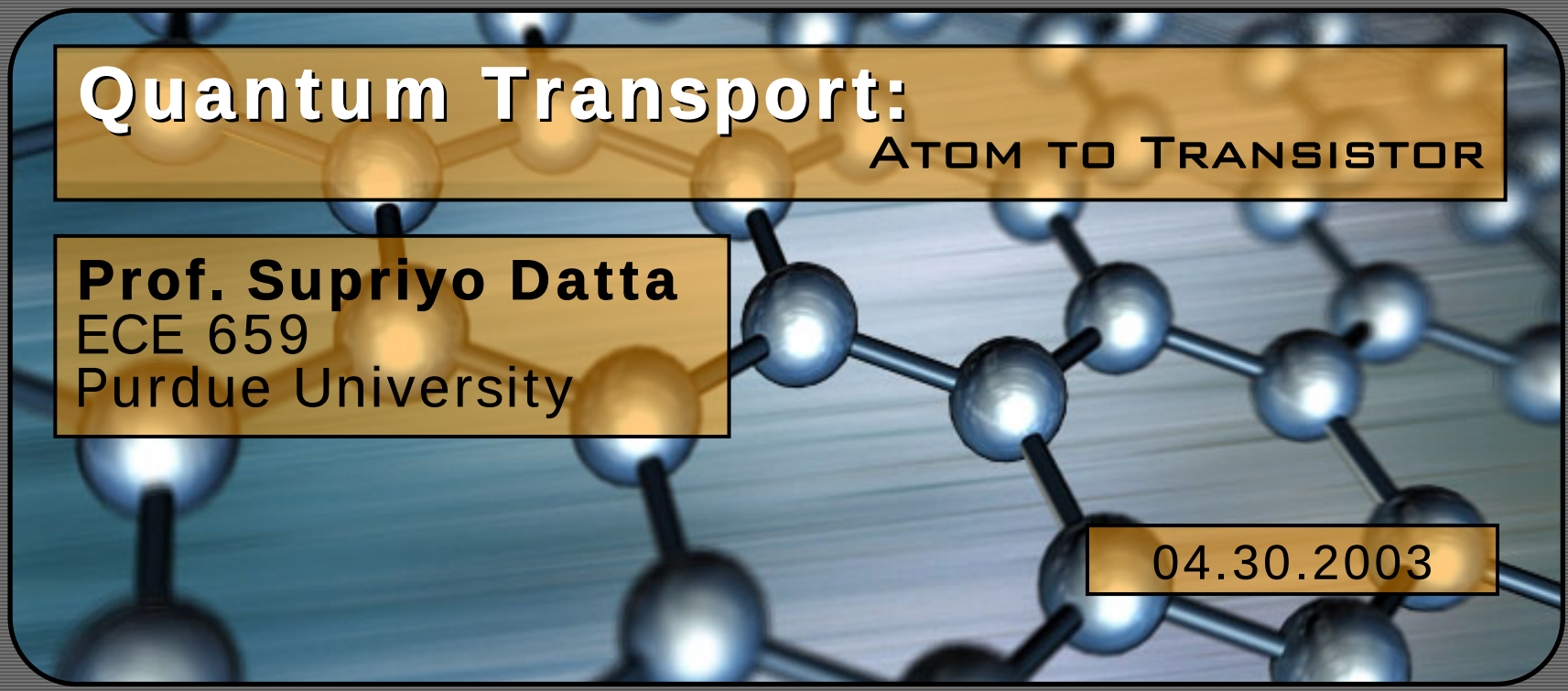

Quantum Transport:
Atom to Transistor

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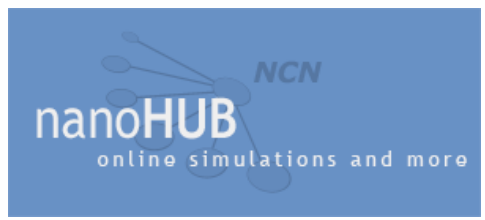
04.30.2003

Lecture 42: Supplementary Topic: Spin

Ref. Chapter 5.4 & 5.5

Network for Computational Nanotechnology



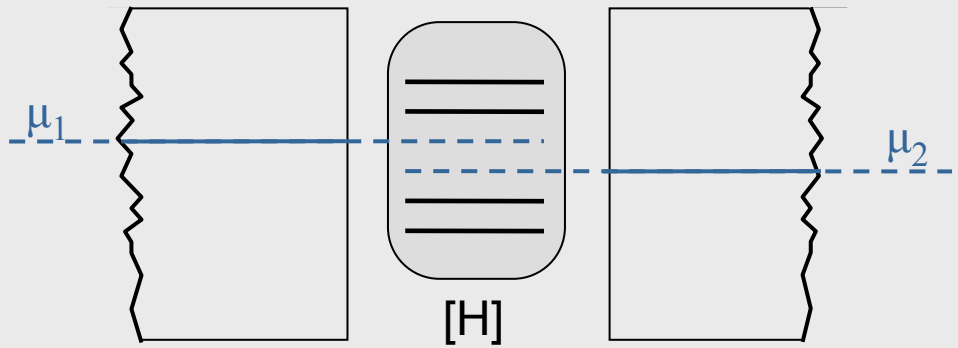
Spin

00:00

• In this lecture, we'll discuss electron spin

• Recall, when deriving current through a small structure, like that show on the right, we first obtain a Hamiltonian [H]. Usually, however, the eigenenergies of [H] represent two degenerate spin levels

Small Device



• The proper Hamiltonian for degenerate spin levels is twice as big

$$\begin{bmatrix} H & O \\ O & H \end{bmatrix}$$

with no coupling between the spin up and spin down portions

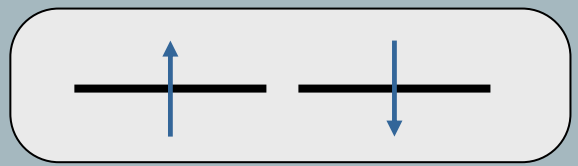
Strong Electron Interactions

02:20

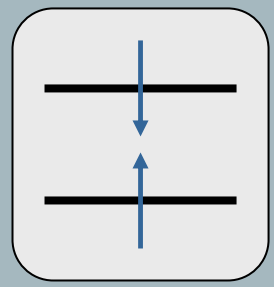
• We want to consider the conditions for which the spin levels are not degenerate. There are two cases by which this arises

• ***Case 1***: Strong Electron-Electron Interactions (i.e. Coulomb Blockade)

→ Because electrons are forced to interact strongly instead of 2 degenerate levels…



… we have two split levels…



the first level fills and forces the second up

→ *Important Example*: Magnetism. All electrons want to have the same spin due to electron-electron interactions.

Spin Orbit Interaction

• ***Case 2***: Spin Orbit Interaction

→ This has nothing to do with electron-electron interactions and is the focus of the remainder of this lecture.

• Continuing with spin-orbit interaction…

Ordinarily the Hamiltonian is

$$\left[\begin{array}{c|c} p^2/2m+U & O \\ \hline O & p^2/2m+U \end{array}\right]$$

• When a magnetic field is applied, say in the $\hat{z}$ direction, up and down spin levels do not remain degenerate so we add

$$\mu_B \begin{bmatrix} B_Z & 0 \\ 0 & -B_Z \end{bmatrix}$$

where μ_B is the Bohr magneton constant $q\hbar/2m$. A well known example of this is the Zeeman effect

Eigenenergies

• If we apply a magnetic field in the x-direction as well the additional term becomes

$$+\mu_B \begin{bmatrix} B_Z & B_X \\ B_X & -B_Z \end{bmatrix}$$

• To summarize, the $\hat{z}$ magnetic field gives

$$\mu_B B_Z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

• … and the $\hat{x}$ magnetic field gives

$$\mu_B B_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

These matrices have the same eigenenergies but different eigenvectors. The eigenenergies are

$+\mu_B B_z$, $-\mu_B B_z$,
$+\mu_B B_x$, $-\mu_B B_x$

Eigenvectors

The eigenvectors are …

$\hat{z}$ direction →

$+\mu_B B_z$ $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$-\mu_B B_z$ $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\hat{x}$ direction →

$+\mu_B B_x$ $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$-\mu_B B_x$ $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Note the different eigenvectors

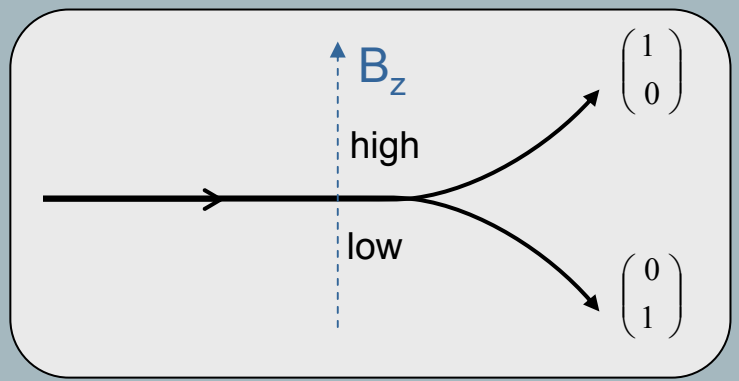
• One might imagine that we could have written the additional term as

$$\mu_B \begin{bmatrix} \sqrt{B_z^2 + B_x^2} & 0 \\ 0 & \sqrt{B_z^2 + B_x^2} \end{bmatrix}$$

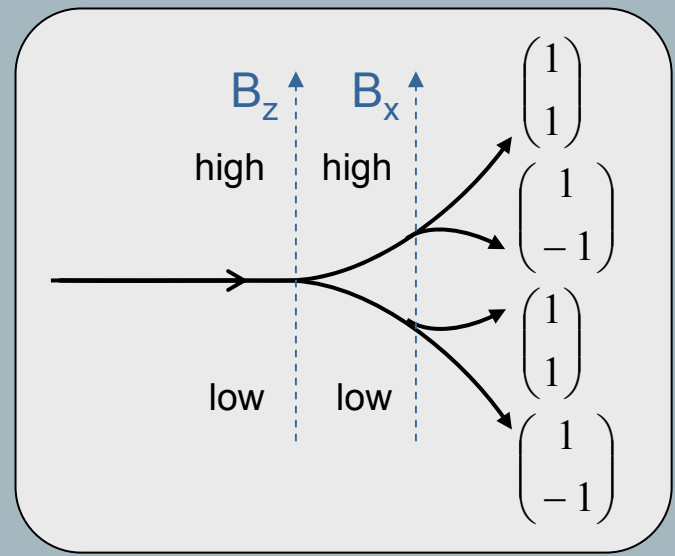
this model does explain the Zeeman effect but fails under what is known as the Stern-Gerlach experiment

Stern-Gerlach Experiment

• In the Stern-Gerlach experiment a beam of electrons is injected into an inhomogeneous magnetic field, due to spin interaction the beam splits after entering the magnetic field.
Example: A beam of electrons split by an inhomogeneous $\hat{z}$ magnetic field



• Example Continued:
And if we add another inhomogeneous, say in the x-direction, the beam splits again



Eigenenergies

• Overall the correct term, valid for any direction, added to the Hamiltonian is

$$\mu_B \begin{bmatrix} B_Z & B_X - iB_y \\ B_X + iB_y & -B_Z \end{bmatrix}$$

Note, regardless of magnetic field direction the splitting effect is the same though the eigenvalues may vary

• Often this matrix is written as $\vec{\sigma} \cdot \vec{B}$

where $\vec{\sigma} = \hat{x}\sigma_x + \hat{y}\sigma_y + \hat{z}\sigma_z$

$$\vec{B} = \hat{x}B_x + \hat{y}B_y + \hat{z}B_z$$

and

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\therefore \vec{\sigma} \cdot \vec{B} = \begin{bmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{bmatrix}$$

Vector Potential

• Moving on we can define spin-orbit interaction…

• Recall, an electric field may be expressed as

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

and a magnetic field as

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

• A scalar potential, U, is simply added into the Schrödinger equation

• But a vector potential, $\vec{A}$, is incorporated as a dot product with the momentum vector $\vec{p}$, i.e.

$$\left[\begin{array}{c|c} \dfrac{\left(\vec{p}+q\vec{A}\right)^2}{2m}+U & 0 \\ \hline 0 & \dfrac{\left(\vec{p}+q\vec{A}\right)^2}{2m}+U \end{array}\right]$$

Spin-Orbit Interaction

• Interestingly, even when there is *no* magnetic field a strong electric field can induce an *effective* magnetic field on an electron. This phenomena occurs due to relativistic interactions between an electron and the applied electric field. Interaction between the electric field of the nucleus and electrons of an atom is a very good example of this. We call this effect “Spin-Orbit Interaction”

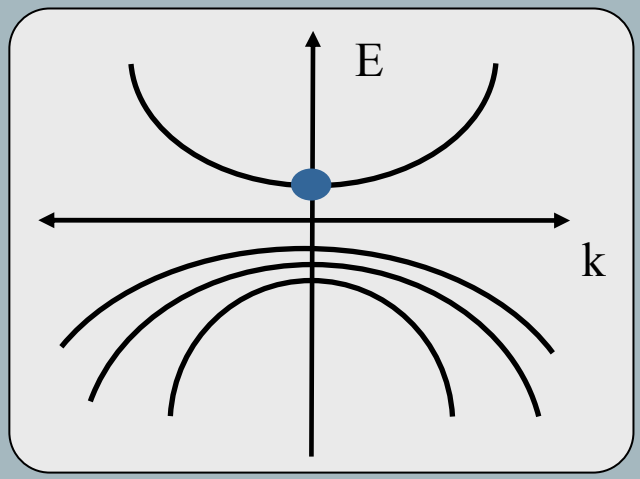
• Spin-Orbit Interaction is incorporated into the system Hamiltonian with the term

$$\mu_B \vec{\sigma} \cdot \left(\frac{\vec{E} \times \vec{p}}{2mc^2} \right)$$

• *Note*: Even in a weak electric field spin-orbit interaction is present but generally is too small to deserve any consideration

Semiconductors

- Spin-Orbit coupling plays a fundamental role in our understanding of semiconductor physics
- Given a semiconductor with an E-k diagram like the following…



- … If we were to examine the area right around the “dot” we would find that conduction band was formed of |s> orbitals and the valence band of |p> orbitals ($|p_x\rangle$,$|p_y\rangle$,$|p_z\rangle$ or in another notation |x>, |y>, |z>)

Isotropic Emission

27:24

- Ignoring spin orbit coupling one might assume semiconductor valence bands of the form |x>, |y>, and |z> separately. If this were the case then a transition from the conduction band, |s>, to say |x> would be polarized in the x direction. Furthermore, since there is no preference in transition to the valence band y-polarized and z-polarized light should be equally likely resulting in overall isotropic emission

- However, this is not the case, emission is not isotropic but in fact circularly polarized. We cannot ignore spin-orbit coupling/interactions. When included, spin-orbit coupling provides an entirely different (but correct) set of valence bands that accurately predict the circularly polarized light emitted from in semiconductors

Correct Valence Bands

29:03

• The first valence band derived with spin-orbit coupling is

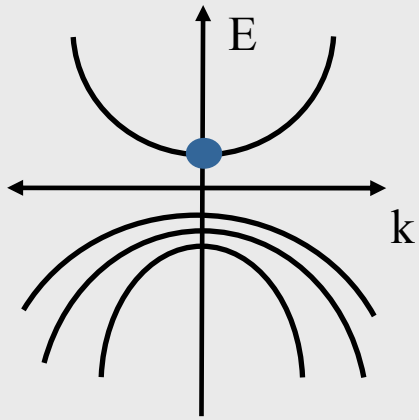
$$\begin{pmatrix} |x\rangle + i|y\rangle \\ 0 \end{pmatrix}$$

and

$$\begin{pmatrix} 0 \\ |x\rangle - i|y\rangle \end{pmatrix}$$

we call this the heavy hole band. We will ignore the other valence bands (light hole) for now since most optical transitions occur to and from the heavy hole band

Heavy Hole Band



• Note: The |s> conduction orbital is not usually affected by spin-orbit coupling

• *Ex*:

$$\begin{pmatrix} |s\rangle \\ 0 \end{pmatrix} \text{ to } \begin{pmatrix} |x\rangle + i|y\rangle \\ 0 \end{pmatrix}$$

will produce circularly polarized light in the x-y plane. So we see what a dramatic physical effect spin-orbit coupling can have

Spin-Orbit Interaction

• *Important Point*: Even when electrons travel at a fraction of the speed of light relativistic phenomena can produce observable effects on spin

• *Note*: In some semiconductors, such as InAs, spin-orbit interaction can alter even the conduction band

• So how does one make sense of the spin-orbit interaction term

$$\mu_B \vec{\sigma} \cdot \left(\frac{\vec{E} \times \vec{p}}{2mc^2} \right)$$

• To begin, look at the vector term in the Hamiltonian (ignoring the spin-orbit term and any scalar potential U):

$$H = \left(\frac{\vec{p} + q\vec{A}}{2m} \right)^2 I + \mu_B \vec{\sigma} \cdot \vec{B}$$

where I is a 2x2 matrix

Vector Hamiltonian

37:00

• Note that

$$\frac{\left(\vec{p}+q\vec{A}\right)^2}{2m} I + \mu_B \vec{\sigma}\cdot\vec{B} \quad (1)$$

is equivalent to

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

where $\vec{\sigma}$ is composed of the Pauli spin matrices

• Furthermore, without any vector potential $\vec{A}$,

$$H = \frac{\left(\vec{\sigma}\cdot\vec{p}\right)^2}{2m} = \begin{bmatrix} p^2/2m & 0 \\ 0 & p^2/2m \end{bmatrix}$$

• But if we include $\vec{A}$ and apply a few dot and cross product identities to ② the familiar $\mu_B\vec{\sigma}\cdot\vec{B}$ term in ① is produced

• *Point*: $\mu_B\vec{\sigma}\cdot\vec{B}$ is related to the general vector Hamiltonian and does not simply appear from nowhere

Deriving the Spin-Orbit Term

39:51

- Now, the spin-orbit interaction term

$$\mu_B \vec{\sigma} \cdot \left(\frac{\vec{\varepsilon} \times \vec{p}}{2mc^2} \right)$$

is relativistic and can only be derived from the full relativistic Hamiltonian

- The full relativistic Hamiltonian, otherwise known as the Dirac equation, is

$$H = \begin{bmatrix} mc^2 I & c\vec{\sigma} \cdot \vec{p} \\ c\vec{\sigma} \cdot \vec{p} & -mc^2 I \end{bmatrix}$$

Note: I is the 2x2 identitiy matrix, c is the velocity of light, and $\vec{p}$ is replaced by $\vec{p} + q\vec{A}$ when a magnetic field is applied

- So how do we get the familiar, low velocity, Schrödinger equation

$$H = \frac{p^2}{2m} I$$

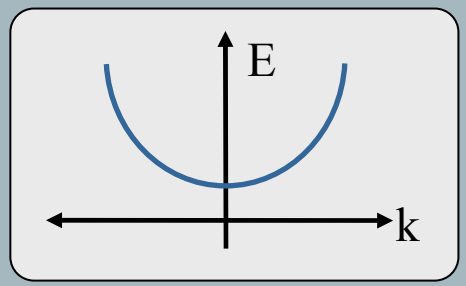
from the Dirac equation?

E-k Relationships

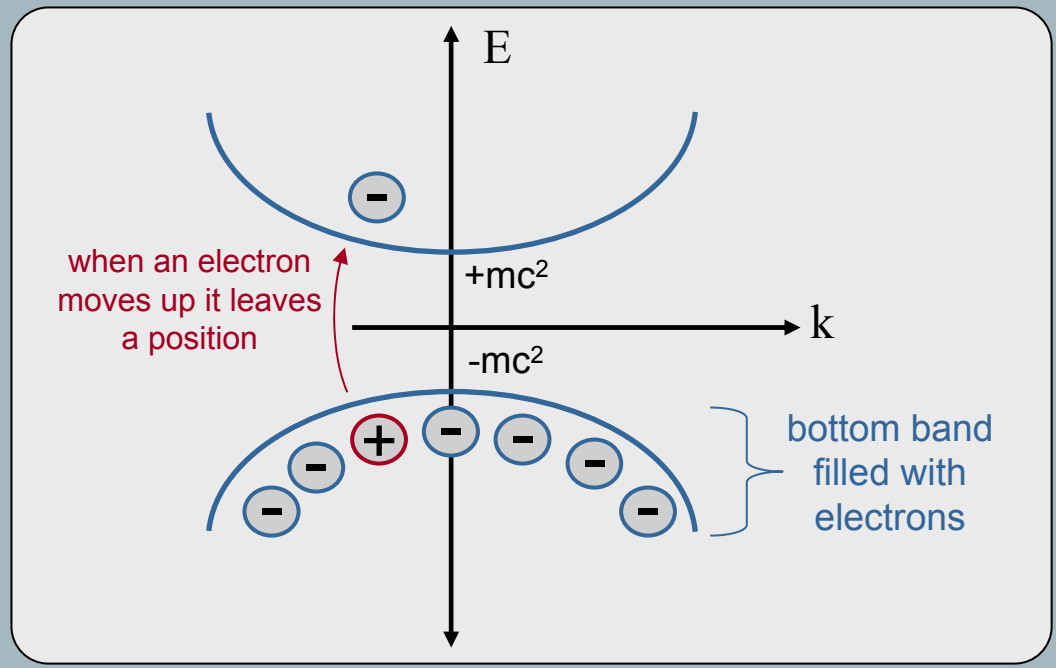
• Recall, the E-k relationship at low electron energies, for which

$$H = \frac{p^2}{2m} I$$

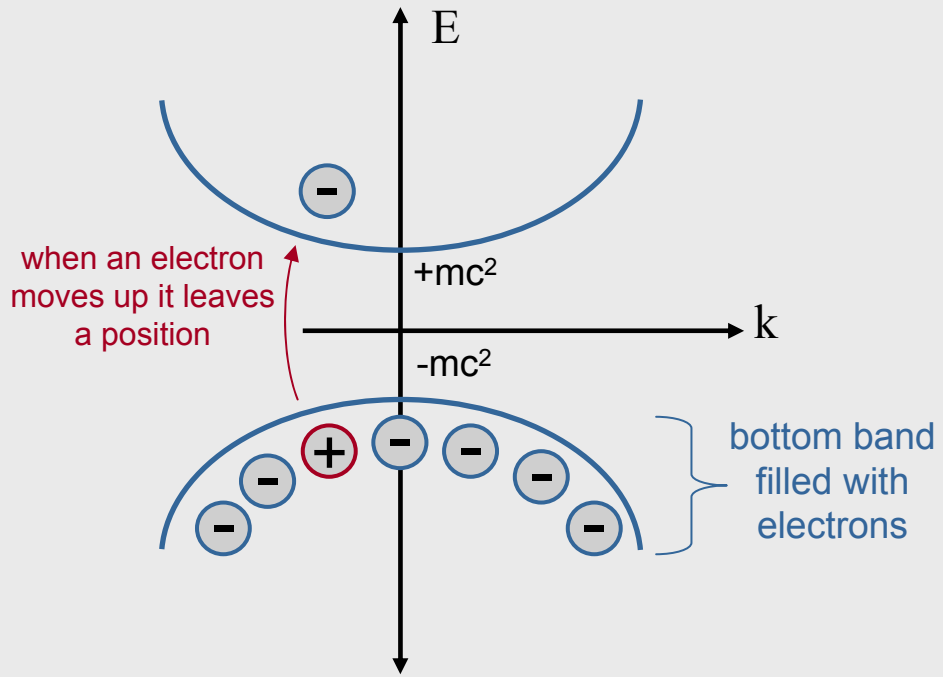
is valid looks like…



• Whereas the high energy Dirac equation produces an E-k relationship of the form…



Only a Few at the Top



• Note however, that moving to the top band requires an energy equal to $2mc^2$ (on the order of 1MeV)

• For the most part, outside high energy experiments, only a few electrons reside in the top-band. Importantly, we can greatly simplify the Dirac equation by concentrating on the few electrons in the top band and ignore the bottom band completely. Based on this assumption we can derive the familiar low energy Hamiltonian.

Dirac Equation Self-Energy

• Conceptually, in the low energy regime we can concentrate on term ① in the Dirac Equation

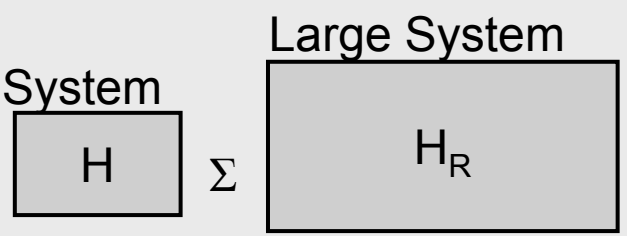
$$\left[\begin{array}{c|c} \overset{①}{mc^2 I} & \overset{②}{c\vec{\sigma}\cdot\vec{p}} \\ \hline \underset{③}{c\vec{\sigma}\cdot\vec{p}} & \underset{④}{-mc^2 I} \end{array}\right]$$

and treat terms ②, ③, and ④ as a self-energy

• Recall, for any system, H, coupled to a larger system, H_R, we may define a self-energy

$$\Sigma = \tau(E - H_R)^{-1}\tau^+$$

Coupled Systems



• For the Dirac equation

$$\tau = c\vec{\sigma}\cdot\vec{p} = \tau^+$$

$$H_R = -mc^2$$

and

$$\Sigma = (c\vec{\sigma}\cdot\vec{p})\left(\frac{1}{E+mc^2}\right)(c\vec{\sigma}\cdot\vec{p})$$

First Order Self-Energy

47:00

• Furthermore, since the electrons we are concentrating on, which lie in the top band, have an energy around mc^2 we may make the approximation $E=mc^2$. Thus,

$$\Sigma = (c\vec{\sigma}\cdot\vec{p})\left(\frac{1}{2mc^2}\right)(c\vec{\sigma}\cdot\vec{p})$$

$$= \frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}$$

• So, overall the non-relativistic first-order Hamiltonian is

$$H = mc^2 I + \frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}$$

• But mc^2I, as constant, may be ignored which gives the familiar

$$H = \frac{(\vec{\sigma}\cdot\vec{p})^2}{2m}$$

• To include spin-orbit interactions we need to improve our approximation for E, that is $E \approx mc^2$, to something more accurate

Closing Comments

• Including a more accurate representation of E complicates the algebra considerably, nonetheless by including a next order approximation of E we are able to derive the familiar spin-orbit interaction term

from the Dirac equation $\mu_B \vec{\sigma} \cdot \left(\frac{\vec{E} \times \vec{p}}{2mc^2} \right)$

• *Main Point*: Spin-orbit interactions, magnetic interaction, vector potentials, etc. all follow from the Dirac equation and are all fundamentally related