Spintronics Note

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Contents

1 The Quantum Mechanics of Spin

1.1 Pauli Matrices

We have the following relations

$$\boxed{\begin{aligned}&[S_i, S_j] = \varepsilon_{ijk} i\hbar S_k \\ &S^2 |s,m\rangle = \hbar^2 s(s+1) |s,m\rangle \\ &S_z |s,m\rangle = \hbar m |s,m\rangle \\ &S_\pm |s,m\rangle = (S_x \pm iS_y) |s,m\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\, |s, m\pm 1\rangle\end{aligned}} \tag{1.1a}$$

We have two states for spin 1/2

$$\alpha = \begin{pmatrix}1\\0\end{pmatrix}; \beta = \begin{pmatrix}0\\1\end{pmatrix}$$

And we can know

$$S^2\alpha = \frac{3}{4}\hbar^2\alpha; S^2\beta = \frac{3}{4}\hbar^2\beta$$

Let $S^2 = \begin{pmatrix}a & b\\ c & d\end{pmatrix}$, then we can get

$$S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

Similarly, we can get

$$S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}; S_+ = \hbar\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}; S_- = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$$

Or

$$S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}; S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}; S_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix};$$

And we let $S = \frac{\hbar}{2}\sigma$, where σ is what we call Pauli Matrix

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

Or to make it easer to remember, we get a generally form

$$\sigma_a = \begin{pmatrix}\delta_{a3} & \delta_{a1} - i\delta_{a2}\\ \delta_{a1} + i\delta a2 & -\delta_{a3}\end{pmatrix}$$

where δ_{ai} is Kronecker delta.

After we get the Pauli matrices, we can correspondingly get their eigenstates which are:

$$\psi_{z+} = \begin{pmatrix}1\\0\end{pmatrix}; \psi_{z-} = \begin{pmatrix}0\\1\end{pmatrix}$$
$$\psi_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}; \psi_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$
$$\psi_{y+} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}; \psi_{y-} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

1.2 The Pauli Equation

We can set the electron' wavefunction as

$$[\psi(\boldsymbol{x})] = \begin{bmatrix}\phi_1(\boldsymbol{x})\\ \phi_2(\boldsymbol{x})\end{bmatrix} \tag{1.2}$$

Where $\boldsymbol{x} = (x, y, z, t)$. Then we can recast the Schrodinger Equation

$$\left(\hat{H} - i\hbar\frac{\partial}{\partial t}[I]\right)[\psi(\boldsymbol{x})] = [0] \tag{1.3}$$

This is a set of two simultaneous differential equations for the two components of the spinor wavefunction–ϕ_1 and ϕ_2. And this is referred to as the *Pauli Equation*.

Right now, we can calculate the expected value of the spin components with special expressions.

$$\langle S_n\rangle = \frac{\hbar}{2}[\psi(\boldsymbol{r},t)]^\dagger\sigma_n[\psi(\boldsymbol{r},t)] \tag{1.4}$$

Specifically,

$$\langle S_x\rangle = \frac{\hbar}{2}\begin{bmatrix}\phi_1^\dagger(\boldsymbol{x}) & \phi_2^\dagger(\boldsymbol{x})\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\phi_1(\boldsymbol{x})\\ \phi_2(\boldsymbol{x})\end{bmatrix} = \hbar Re(\phi_1^\dagger(\boldsymbol{x})\phi_2(\boldsymbol{x})) \tag{1.5}$$

$$\langle S_y\rangle = \hbar Im(\phi_1^\dagger(\boldsymbol{x})\phi_2(\boldsymbol{x})) \tag{1.6}$$

$$\langle S_z\rangle = \hbar(|\phi_1(\boldsymbol{x})|^2 - |\phi_2(\boldsymbol{x})|^2) \tag{1.7}$$

1.3 Dirac Equation

Well, Pauli's theory about spin is non-relativistic. The task is finished by Paul Dirac with his Relativistic Wave Equation.

1.3.1 Klein-Gordon Equation

As soon as Schrodinger equation was proposed, the relativistic wave equation was also put forward. That is Klein-Gordon Equation

$$-\hbar^2\frac{\partial^2}{\partial t^2}\psi = (-\hbar^2c^2\boldsymbol{\nabla}^2 + m^2c^4)\psi$$

But this equation can not describe one-single particle, instead it can be used to describe a field–scalar field. The reason mainly comes from the second derivative respect to time. Well let's see the details.

For non-relativistic case, we have equation

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi$$

And we can set

$$\rho = \psi^\star\psi$$

$$\boldsymbol{j} = -\frac{i\hbar}{2m}(\psi^\star\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^\star) = \frac{\langle p\rangle}{m}$$

Then we can get one equation

$$\boxed{\frac{\partial}{\partial t}\rho + \boldsymbol{\nabla}\cdot\boldsymbol{j} = 0}$$

Now, let's prove this, first we have one equation

$$-i\hbar\frac{\partial}{\partial t}\psi^\star = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi^\star$$

Then we take

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}(\psi^\star\psi) &= i\hbar(\dot{\psi}^\star\psi + \psi^\star\dot{\psi}) \\ &= \frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi^\star\psi - \frac{\hbar^2}{2m}\psi^\star\boldsymbol{\nabla}^2\psi \\ &= \frac{\hbar^2}{2m}\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\psi^\star\psi - \psi^\star\boldsymbol{\nabla}\psi) \end{aligned}$$

Finally, we can get

$$\begin{gathered} \frac{\partial}{\partial t}(\psi^\star\psi) = -\frac{i\hbar}{2m}\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\psi^\star\psi - \psi^\star\boldsymbol{\nabla}\psi) \\ \Downarrow \\ \frac{\partial}{\partial t}\rho = -\boldsymbol{\nabla}\cdot\boldsymbol{j} \end{gathered}$$

This is actually the conversation of probability. Well but this is not very true for Klein-Gordon Equation. With the same way, we can have

$$-\hbar^2\frac{\partial}{\partial t}(\psi^\star\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^\star) = -\hbar^2c^2\boldsymbol{\nabla}\cdot(\psi^\star\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^\star)$$

Now we need to re-set the symbols

$$\rho = \frac{i\hbar}{2mc^2}(\psi^\star\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^\star)$$

$$\boldsymbol{j} = -\frac{i\hbar}{2m}(\psi^\star\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^\star)$$

We can still get

$$\frac{\partial}{\partial t}\rho + \boldsymbol{\nabla}\cdot\boldsymbol{j} = 0$$

Well, we still get a equation looks like the conversation of probability equation. But here has some difference. What is the meaning of ρ here, it can't be seen as probability density simply. And it's not always positive. Well this "minuse probability" problem can't be solved when we treat Klein-Gordon Equation as suitable relativistic wave equation. Then Dirac mentioned an equation named after him.

1.3.2 Dirac Equation

Klein-Gordon Equation can be written as

$$\Big[(i\hbar\frac{\partial}{c\partial t})^2-\sum_1^3(-i\hbar\frac{\partial}{\partial x_r})^2-m_0^2c^2\Big]\psi(x,y,z,t)=0$$

When there is a field $\vec{A}=(A_0,A_x,A_y,A_z)$, the equation will become

$$\Big[(i\hbar\frac{\partial}{c\partial t}+eA_0)^2-\sum_1^3(-i\hbar\frac{\partial}{\partial x_r}+eA_r)^2-m_0^2c^2\Big]\psi(x,y,z,t)=0$$

Well, Dirac think the relativistic wave equation should also be first order differential respect to time. According to the relativity, time and coordinates have the same status, so the equation should also be first order differential respect to coordinate. Finally, he thought the right form should be

$$\Big[(i\hbar\frac{\partial}{c\partial t}+eA_0)-\sum_1^3\alpha_r(-i\hbar\frac{\partial}{\partial x_r}+eA_r)-\alpha_0m_0^2c^2\Big]\psi(x,y,z,t)=0$$

On the other hand, for a free particle we have known

$$E^2=p^2c^2+m_0^2c^2$$

2 Magneto-Electric Subbands in Quantum Confined Structures in the presence of Spin-Orbit Interaction

When an electron is confined in a structure of restricted dimensionality(such as quantum well or a quantum wire) and is subjected to a magnetic field, the electron experiences both electrostatic confinement due to structure and magnetostatic confinement due to the magnetic field. Aa a result, the allowed electronic states are hybrid magneto-electric states which form a subbands. In this chapter, we will derive the dispersion relations in these subbands in the presence of SOC.

2.1 Spin-Orbit-Interaction in a Solid

According to a well know discussion, we can get nuclear attracted electron's SOC

$$H_{SO} = -\frac{g_e e\hbar}{8m^2c^2}(\nabla V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma} = -\frac{e\hbar}{4m^2c^2}(\nabla V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma} \tag{2.1}$$

Where $\boldsymbol{\sigma}$ is pauli matrices.

In a solid, a quasi-free electron in the conduction band does not experience the strong nuclear attraction as in an atom. However, it may still see an electric field(or potential gradient) due to internal effects such as the discontinuity of the conduction band in a heterostructure or due to an externally applied E-field. And this field will induce a SOC with the form of Hamiltonian 2.1.

There are two types SOC in Solid which can be classified according to two different inversion asymmetries. First is *Structual Inevrsion Asymmetry(SIA)* and the corresponding Rashba Interaction. Second is *Crystallographic Inversion Asymmetry* and Dresselhaus Interaction.

而Rashba效应和Dresselhaus效应主要区别是产生等效磁场的的电场的来源不同：Rashba效应主要发生在二维体系，如二维原子层或者是异质结表面某种原因所带来的中心反演对称性破缺带来的；Dersselhaus效应主要是发生在三维体系，主要是材料本身原子晶格的不对称性带来的中心反演对称性的破缺而引起的。Zeeman效应则是由于外加的宏观磁场产生的自旋的极化方向平行或者反平行于磁场方向所带来的劈裂。

2.1.1 Rashba Interaction

For a crystal electron, we can have

$$H_{SO}^{band} = \frac{ge\hbar}{8(m^\star)^2c^2}\nabla V \cdot (\boldsymbol{\sigma} \times \boldsymbol{p}) = -\frac{ge\hbar}{8(m^\star)^2c^2}\boldsymbol{E} \cdot (\boldsymbol{\sigma} \times \boldsymbol{p})$$

Where $m^\star$ is the effective mass. And the Rashba interaction is almost the same form with

$$H_R = -\boldsymbol{\eta}_R \cdot (\boldsymbol{\sigma} \times \boldsymbol{p}) \tag{2.2}$$

$$\boldsymbol{\eta}_R = -\frac{ge\hbar}{8(m^\star)^2c^2}\boldsymbol{E}(\boldsymbol{r}) \tag{2.3}$$

This is the simplistic form, after we consider the band structure effects in a solid, we will get

$$\boldsymbol{\eta}_R = -\frac{e\hbar}{m^\star(\vec{r})}\frac{\pi\Delta_s(2E_g+\Delta_s)}{E_g(E_g+\Delta_s)(3E_g+2\Delta_s)}\boldsymbol{E}(\vec{r}) \tag{2.4}$$

Where E_g is the band gap of and Δ_s is the spin-orbit splitting in the valance band. On the other hand, if there is also magnetic field, we need to re-write our expression with $\boldsymbol{p} + e\boldsymbol{A}$ instead of $\boldsymbol{p}$.

$$H_R = \boldsymbol{\eta}_R(\vec{r}) \cdot [\boldsymbol{\sigma} \times (\boldsymbol{p} + e\boldsymbol{A})]$$

2.1.2 Dresselhaus Interaction

The Pauli Equation 1.3 describe a single electrons in a crystal lattice in the absence of any external magnetic field, but in the presence of SOC the equation will become

$$\Big[\frac{\boldsymbol{p}^2}{2m_0} + V_{lattice} - \frac{e\hbar}{4m_0^2c^2}(\boldsymbol{\nabla} V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma}\Big][\psi] = E[\psi] \tag{2.5}$$

Where $V_{lattice}$ is the (spatially periodic) electrostatic potential energy due to the ionized atoms in the crystal. And we have the wavefunction should follow Bloch theorem

$$[\psi] = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}[u_{\boldsymbol{k}}(\vec{r})] = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \begin{bmatrix} u_{\boldsymbol{k}}^{\uparrow}(\vec{r}) \\ u_{\boldsymbol{k}}^{\downarrow}(\vec{r}) \end{bmatrix}$$

Then we can re-write equation 2.5 with substituting the upper Bloch form

$$\begin{aligned}\Big[\frac{\boldsymbol{p}^2}{2m_0} + V_{lattice} - \frac{e\hbar}{4m_0^2c^2}(\boldsymbol{\nabla} V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma}\Big][u_{\boldsymbol{k}}(\vec{r})] \\ + \hbar\boldsymbol{k} \cdot \Big[\frac{p}{m_0} - \frac{e\hbar}{4m_0^2C^2}(\boldsymbol{\sigma} \times \boldsymbol{\nabla} V)\Big][u_{\boldsymbol{k}}(\vec{r})] = (E_k - \frac{\hbar^2k^2}{2m_0})[u_{\boldsymbol{k}}(\vec{r})]\end{aligned}$$

The similar equation should be the next expression for $\boldsymbol{k} + \boldsymbol{K}$ with $\boldsymbol{K}$ is the reciprocal lattice vector

$$\begin{aligned}\Big[\frac{\boldsymbol{p}^2}{2m_0} + V_{lattice} - \frac{e\hbar}{4m_0^2c^2}(\boldsymbol{\nabla} V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma}\Big][u_{\boldsymbol{k}+\boldsymbol{K}}(\vec{r})] \\ + \hbar\boldsymbol{k} \cdot \Big[\frac{p}{m_0} - \frac{e\hbar}{4m_0^2C^2}(\boldsymbol{\sigma} \times \boldsymbol{\nabla} V)\Big][u_{\boldsymbol{k}+\boldsymbol{K}}(\vec{r})] \\ + \hbar\boldsymbol{K} \cdot \Big[\frac{p}{m_0} - \frac{e\hbar}{4m_0^2C^2}(\boldsymbol{\sigma} \times \boldsymbol{\nabla} V)\Big][u_{\boldsymbol{k}+\boldsymbol{K}}(\vec{r})] = (E_k - \frac{\hbar^2(\boldsymbol{k}+\boldsymbol{K})^2}{2m_0})[u_{\boldsymbol{k}+\boldsymbol{K}}(\vec{r})]\end{aligned}$$

With treating the term $\hbar\boldsymbol{K} \cdot \Big[\frac{p}{m_0} - \frac{e\hbar}{4m_0^2C^2}(\boldsymbol{\sigma} \times \boldsymbol{\nabla} V)\Big]$ as a perturbation ad applying group theoretic results, Dresselhaus derived the SOC Hamiltonian and spin-splitting energies in principal crystallographic directions. And for this direction, it has the form

$$H_D = \nu_D \boldsymbol{\sigma} \cdot \boldsymbol{\kappa} \tag{2.6}$$

Where

$$\kappa_i = \frac{1}{2\hbar^3}\delta_{ijk}[p_i(p_j^2 - p_k^2) + (p_j^2 - p_k^2)p_i]^1$$

Right now we can see the scheme

[1] $k_x = \frac{1}{2\hbar^3}[p_x(p_y^2 - p_z^2) + (p_y^2 - p_z^2)p_x]$

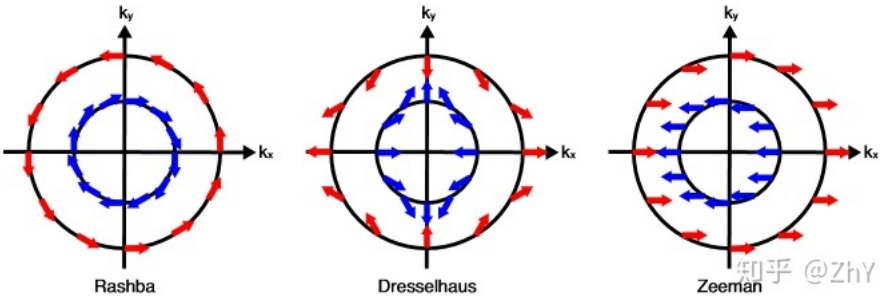

Figure 1: Two types SOC and Zeeman Effect to show the spin and momentum.

2.2 Magneto-electric subbands in a 2D electron gas in the presence of spin-orbit interaction

The general form of Hamiltonian for 2DEG moving in magneto-electric field should be

$$H_{2DEG} = \frac{|\vec{p} + e\vec{A}|^2}{2m^\star} + V(z) + H_Z + H_R + H_D \tag{2.7}$$

Where H_z is Zeeman interaction, H_R, H_D are Rashba and Dresselhaus effect. $V(z)$ comes from the electrostatic potential in z direction. (Typically, this potential comes from the band discontinuity at the hetero-interface or external applied E-field).

The key to solve this hamiltonian is to know the fields. Next we will introduce some systems.

2.2.1 Magnetic field in the plane of the 2DEG

We apply

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

Then we can get

$$\begin{aligned} H^{||}_{2DEG} =& \frac{1}{2m^\star}[(p_x + eB_y z)^2 + (p_y - eB_x z)^2 + p_z^2] + V(z) \\ & - \frac{g}{2}\mu_B[B_x\sigma_x + B_y\sigma_y] - \frac{\eta_R}{\hbar}[(p_x + eB_y z)\sigma_y - (p_y - eB_x z)\sigma_x] \\ & + H_D \end{aligned} \tag{2.8}$$

Well, $||$ reminds there is a magnetic field parallel to the plane of 2DEG. here H_D is a little complex cause it has many terms. But we can use one approximation which is $\langle p_z\rangle^2 >> \langle p_x\rangle^2, \langle p_y\rangle^2$. Cause in the material, when we use 2DEG model, the perpendicular direction should be uniform, in the other words, the vertical momentum should be much larger than the transverse ones. With this we can get

$$H_D = -\frac{\nu_D}{\hbar^3}p_z^2[(p_x + eB_y z)\sigma_x - (p_y - eB_x z)\sigma_y]$$

With Pauli Equation

$$[H^{||}_{2DEG}][\psi^{||}_{2DEG}(x,y,z)] = E[\psi^{||}_{2DEG}(x,y,z)]$$

Where $[H^{||}_{2DEG}]$ is a 2×2 matrix and $[\psi^{||}_{2DEG}(x,y,z)]$ is the 2-component wavefunction. We can easily see $H^{||}_{2DEG}$ is x,y dependent freely, so we can write that

$$\psi^{||}_{2DEG} = e^{ikx}e^{iky}\lambda(z)$$

And then the the Pauli equation taken detailed form becomes

$$\begin{aligned}&\Big\{\frac{\hbar^2k_x^2}{2m^\star}+\frac{\hbar^2k_y^2}{2m^\star}-\frac{\hbar^2}{2m^\star}\frac{\partial^2}{\partial z^2}+V(z)+eB_yz\frac{\hbar k_x}{m^\star}eB_xz\frac{\hbar k_y}{m^\star}+e^2z^2\frac{B_x^2+B_y^2}{2m^\star}\\ &-\frac{g}{2}\mu_B(B_x\sigma_x+B_y\sigma_y)-\frac{\eta_R}{\hbar}[(\hbar k_x+eB_yz)\sigma_y-(\hbar k_y-eB_xz)\sigma_x]\\ &-\frac{\nu_D}{\hbar^3}p_z^2[(p_x+eB_yz)\sigma_x-(p_y-eB_xz)\sigma_y]\Big\}[\lambda(z)]=E[\lambda(z)]\end{aligned}$$

Where the boundary condition should be

$$[\lambda(z)](z=d)=[\lambda(z)](z=-d)=[0] \tag{2.9}$$

Well here we assume a infinite rectangular potential wall located at $z=d/-d$. If the height of wall is finite, the problem should be much more complicated. On the other hand, we first should set given values of k_y and E, then the dispersion relation related on k_x can be obtained, vice versa for k_y. Finally, a two variables dependent $E(\boldsymbol{k}_x,\boldsymbol{k}_y)$ can be acquired.

But the procedure is not easy because the upper Pauli equation is not a linear equation for k_x,k_y which means it's not an eigen-equation for both $\boldsymbol{k}$. So the first step is to convert this equation to an eigen-equation with the expression

$$[\varsigma(z)]=k_x[\lambda(z)] \tag{2.10}$$

Then we get

$$\{\boldsymbol{B}k_x+\boldsymbol{C}\}[\lambda(z)]=\boldsymbol{A}k_x^2[\lambda(z)] \tag{2.11}$$

With

$$\begin{aligned}\boldsymbol{A}&=-\frac{\hbar^2}{2m^\star}\boldsymbol{I}\\ \boldsymbol{B}&=eB_yz\frac{\hbar}{m^\star}\boldsymbol{I}-\eta_R[\sigma_y]-\nu[\sigma_x]\\ \boldsymbol{C}&=\frac{\hbar^2k_y^2}{2m^\star}\boldsymbol{I}-\frac{\hbar^2}{2m^\star}\frac{\partial^2}{\partial z^2}\boldsymbol{I}-eB_xz\frac{\hbar k_y}{m^\star}\boldsymbol{I}+V(z)\boldsymbol{I}+\underbrace{\cdots\cdots}_{\text{complex}}\end{aligned}$$

3 Spin Torques