Spintronics Note

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Contents

1 The Quantum Mechanics of Spin

1.1 Pauli Matrices

We have the following relations

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

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

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

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. 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

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

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