Derivation and Characteristics of Geometric Phases in Quantum Mechanics

Introduction to Berry Phase

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Phase of wave function

Wave function $\psi(\boldsymbol{r}, t)$

Wave function is complex number

$|\psi|^2$ Existence probability

$$\psi = |\psi| e^{i\theta}$$

Absolute term phase term

Absolute value of the wave function is observable

Phase of wave function is not observable

phase is not appear in physics phenomena?

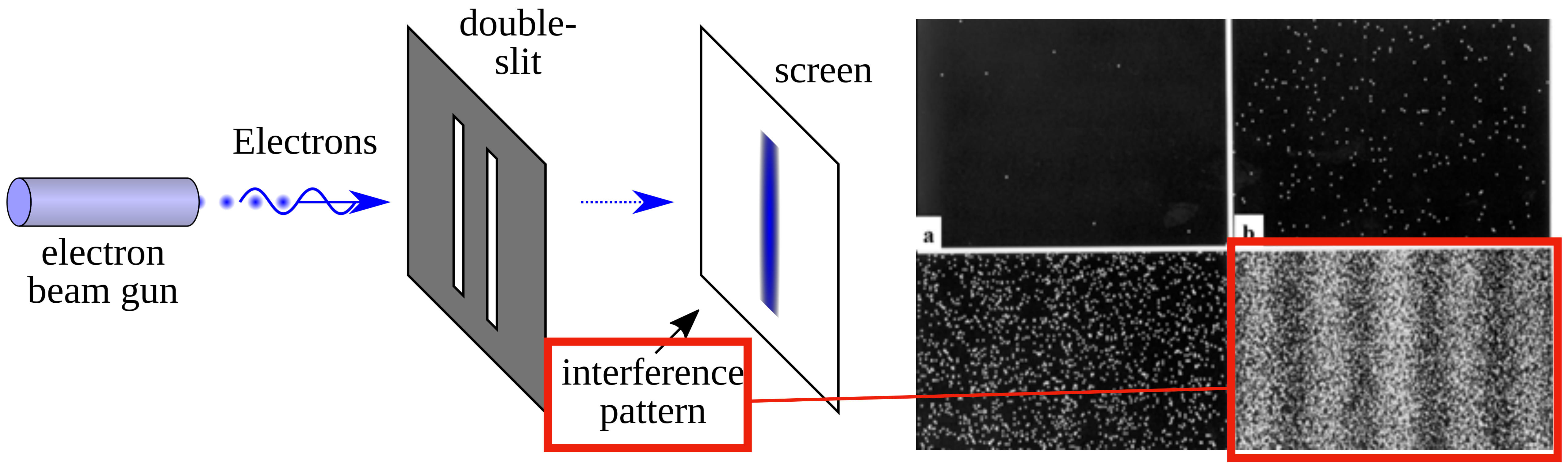
→ It is appear in case of the condition..

Principle of superposition

$$\psi = \psi_1 + \psi_2 = |\psi_1| e^{i\theta_1} + |\psi_2| e^{i\theta_2}$$
$$\rightarrow |\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2| cos(\theta_1 - \theta_2)$$

Phase differences can be observable!!

Example: Double slit experiment -> wave nature of electrons



Point

Phase of wave function is observable in case of superposition!!

(Difference in phase of wave functions at the same point)

Gauge transformation

The phase of the wave function has degrees of freedom

$$\psi_1 = |\psi_1|e^{i\theta_1} \rightarrow |\psi_1|^2 = |\psi_1|^2$$ → θ_1 is vanished!

$$\psi_2 = |\psi_2|e^{i\theta_2} \rightarrow |\psi_2|^2 = |\psi_2|^2$$ → θ_2 is vanished!

$$\psi = \psi_1 + \psi_2 = |\psi_1|e^{i\theta_1} + |\psi_2|e^{i\theta_2}$$

$$\rightarrow |\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2|cos(\theta_1 - \theta_2)$$ → $\theta_1 - \theta_2$ is not vanished!

Important on physics is differences of phase.

Local gauge transformation

$$\psi(\vec{r}) \rightarrow \psi'(\vec{r}) = \psi(\vec{r})e^{i\theta(\vec{r})}$$ → ψ, ψ' are same mean in physics

Gauge transformation

Introducing Vector Potentials

problem

Momentum is not a gauge invariant…

$$\langle\psi'|\hat{p}_i|\psi'\rangle = \langle\psi|\hat{p}_i|\psi\rangle + \hbar\langle\psi|\frac{\partial\theta}{\partial r_i}|\psi\rangle$$

→ check it!

Solution strategy

Add another term to make it observable

$$\hat{\boldsymbol{P}} + e\boldsymbol{A}$$

$$\begin{cases} -e\ (e>0) & \text{electron charge} \\ \boldsymbol{A} & \text{vector potential} \end{cases}$$

Gauge transformation

$$\begin{cases} \psi'(\vec{r}) = \psi(\vec{r})e^{i\theta(\boldsymbol{r})} \\ \boldsymbol{A}'(\boldsymbol{r}) = \boldsymbol{A}(\boldsymbol{r}) - \frac{\hbar}{e}\nabla\theta(\boldsymbol{r}) \end{cases}$$

→ check it!

$$\langle\psi'|\hat{p}_i + eA'_i|\psi'\rangle = \langle\psi|\hat{p}_i + eA_i|\psi\rangle$$ ➡ gauge invariant

Connection and Curvature

In physics, gauge field, gauge strength

$$\nabla \times \boldsymbol{A} = \boldsymbol{B} \quad \begin{cases} \boldsymbol{A} & \text{: gauge filed, connection (in electro-magnetism it is called vector potential)} \\ \boldsymbol{B} & \text{: gauge strength, curvature (in electro-magnetism it is called magnetic field)} \end{cases}$$

Gauge invariance

$$\begin{cases} \boldsymbol{A}' = \boldsymbol{A} - \frac{\hbar}{e}\nabla\theta \\ \boldsymbol{B}' = \boldsymbol{B} \end{cases}$$

$\boldsymbol{A}'$ → Not observable

$\boldsymbol{B}'$ → observable! → check it!

Consider the line integral of a closed curve

$$\oint_C \boldsymbol{A} \cdot d\boldsymbol{r}$$

→ observable! → check it!

$$\oint_C \boldsymbol{A} \cdot d\boldsymbol{r} = \int_S \nabla \times \boldsymbol{A} \cdot d\boldsymbol{S} = \int_S \boldsymbol{B} \cdot d\boldsymbol{S}$$

Next Seminar…

Introduction Berry pahse

- Monopole
- Berry phase,Berry connection, Berry curvature…(in general parameter)
- Berry phase,Berry connection, Berry curvature…(in wave space)
- Hall effect and Berry curvature.

Don't miss it!

Progress report

Analyse energy band structure Janus transition metal dichalcogenide

- Calculate energy band structure and PDOS janus TMDC (WSSe) on DFT(Q.E).
- Make pannier function (wannier90)
- Plot band structure on tight binding model
- Calculate optical conductivity.

DFT (Q.E) energy band structure and PDOS