Gauge Transformation and Symmetry of Wavefunction: Aharonov-Bohm Effect

In general, symmetry in quantum mechanics stems entirely from microscopic observations that keep the rough scales of atoms and molecules in mind. In much larger systems such as solid, the phase of electron wavefunction breaks under the influence of inelastic scattering caused by thermal vibration of lattice. Phases of electron wavefunction plays very essential roles in quantum mechanical phenomena, but which is hardly observed at macroscopic scale except for the phenomena such as superconductivity and superfluidity. However, it is now possible to observe the quantum mechanical phenomena where the "phase" plays an essential role, under mesoscopic scale (systems between microscopic and macroscopic scales). Let us now explain of a typical phenomenon in which the phase of wavefunctions play an essential role.

Interference of Electron Waves and Aharonov-Bohm Effect

Let's consider an electron in the uniform electromagnetic field in space. The Hamiltonian in this system can be written as following ($-e$ is an electric charge of an electron):

$$H = \frac{1}{2m}(\boldsymbol{p} + e\boldsymbol{A})^2 + V(\boldsymbol{r}) - e\phi(\boldsymbol{r}) \tag{1}$$

$\boldsymbol{A}$ and ϕ represent vector potential and scalar potential respectively, and the relation between the electric field $\boldsymbol{E}$ and magnetic flux density $\boldsymbol{B}$ in the system is given:

$$\boldsymbol{E} = -\frac{\partial \boldsymbol{A}}{\partial t} - \mathrm{grad}\phi \tag{2}$$

$$\boldsymbol{B} = \mathrm{rot}\,\boldsymbol{A} \tag{3}$$

Remember that the equation (1) is derived by Lorenz force as a starting point:

$$\boldsymbol{F} = -e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \tag{4}$$

Normally, $\boldsymbol{E}$ and $\boldsymbol{B}$ are the entity of electromagnetic field so that $\boldsymbol{A}$ and ϕ should be considered simply as a convenient means of support. The vector potential $\boldsymbol{A}$ and the scalar potential ϕ cannot be fixed completely, as we can transform these potentials by using arbitrary scalar function $\chi(\boldsymbol{r}, t)$ to obtain the following:

$$\boldsymbol{A} \to \boldsymbol{A} = \boldsymbol{A}' + \mathrm{grad}\chi$$

$$\phi \to \phi = \phi' - \frac{\partial \chi}{\partial t} \tag{5}$$

We still find the same electric field and magnetic flux density after the transformation:

$$\boldsymbol{E} = -\frac{\partial}{\partial t}(\boldsymbol{A}' + \mathrm{grad}\chi) - \mathrm{grad}(\phi' - \frac{\partial \chi}{\partial t}) = -\frac{\partial \boldsymbol{A}'}{\partial t} - \mathrm{grad}\phi' = \boldsymbol{E}$$

$$\boldsymbol{B} = \mathrm{rot}(\boldsymbol{A}' + \mathrm{grad}\chi) = \mathrm{rot}\,\boldsymbol{A}' + \mathrm{rot}\cdot\mathrm{grad}\chi = \mathrm{rot}\,\boldsymbol{A}' = \boldsymbol{B}'$$

The transformation (5) is called "gauge transformation". In the electromagnetic field, $\boldsymbol{E}$ and $\boldsymbol{B}$ are observed to stay the same after conducting the gauge transformation (5). Now, what do we find for the wavefunction of the electron after the gauge transformation? We suppose $\psi(\boldsymbol{r},t)$ as solution for Schrodinger's equation of Hamiltonian (1):

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t)=[\frac{1}{2m}\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}(\boldsymbol{r},t)\}^2+V(\boldsymbol{r})-e\phi(\boldsymbol{r},t)]\psi(\boldsymbol{r},t) \tag{6}$$

While a solution for the gauge transformation we suppose $\psi'(\boldsymbol{r},t)$:

$$i\hbar\frac{\partial}{\partial t}\psi'(\boldsymbol{r},t)=[\frac{1}{2m}\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}'(\boldsymbol{r},t)\}^2+V(\boldsymbol{r})-e\phi'(\boldsymbol{r},t)]\psi'(\boldsymbol{r},t) \tag{6'}$$

ψ and ψ' are the wavefunctions that are combined by the gauge transformation. To test this, let's derive $u(\boldsymbol{r},t)$ with following:

$$\psi'(\boldsymbol{r},t)=\psi(\boldsymbol{r},t)u(\boldsymbol{r},t) \tag{7}$$

We can use ψ and u to rewrite the quantity concerning with wavefunction after transformation is conducted:

$$\{i\hbar\frac{\partial}{\partial t}+e(\phi+\frac{\partial\chi}{\partial t})\}\psi'=u\{i\hbar\frac{\partial}{\partial t}+e\phi\}\psi+\psi\{i\hbar\frac{\partial u}{\partial t}+eu\frac{\partial\chi}{\partial t}\}\ ,$$

$$\{\frac{\hbar}{i}\nabla+e(\boldsymbol{A}-e\cdot\mathrm{grad}\chi)\}\psi'=u\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}\psi+\psi\{\frac{\hbar}{i}(\nabla u)-eu(\nabla\chi)\}$$

Moreover,

$$\begin{aligned}
&\{\frac{\hbar}{i}\nabla+e(\boldsymbol{A}-e\cdot\mathrm{grad}\chi)\}^2\psi'\\
&\quad=\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}u\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}\psi+\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}\psi\{\frac{\hbar}{i}(\nabla u)-eu(\nabla\chi)\}\\
&\qquad-e(\nabla\chi)\cdot u\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}\psi-e(\nabla\chi)\cdot\psi\{\frac{\hbar}{i}(\nabla u)-eu(\nabla\chi)\}\\
&\quad=u\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}^2\psi+2(\{\frac{\hbar}{i}\nabla+e\boldsymbol{A}\}\psi)\cdot(\{\frac{\hbar}{i}\nabla-e(\nabla\chi)\}u)\\
&\qquad+\psi\{\frac{\hbar}{i}\nabla-e(\nabla\chi)\}^2u\ ,
\end{aligned}$$

In the equation above, ∇ within the parentheses do not operate to the functions outside. To substitute the above into the equation (6'), if we can obtain the solution $u(\boldsymbol{r},t)$ satisfying the followings, then the solution for Schrodinger's equation (6') can be obtained in the same way in (7):

$$\begin{aligned}
&i\hbar\frac{\partial u}{\partial t}+eu\frac{\partial\chi}{\partial t}=0\\
&\frac{\hbar}{i}\nabla u-eu(\nabla\chi)=0
\end{aligned} \tag{8}$$

Above equations simply yield the solution:

$$u = \exp\{+i\frac{e}{\hbar}\chi(\boldsymbol{r},t)\} \tag{9}$$

Therefore, (7)(9) implies that in conducting the gauge transformation (5), wavefunction of electron is transformed to be:

$$\psi'(\boldsymbol{r},t) = \psi(\boldsymbol{r},t)\exp\{+i\frac{e}{\hbar}\chi(\boldsymbol{r},t)\} \tag{10}$$

Schrodinger's equation is written in exact the same way before transformation by using transformed vector potential, scalar potential, and wavefunction.

Let us now go back to study whether the electrons sense $\boldsymbol{E}$ and $\boldsymbol{B}$, or rather sense $\boldsymbol{A}$ and ϕ. Aharonov and Bohm drew attention to this problem and eventually demonstrated that the real field is depending on vector potential $\boldsymbol{A}$ and scalar vector ϕ. The phenomenon in which an electron is affected by $\boldsymbol{A}$ and ϕ to produce the interference pattern of wavefunction is called Aharonov-Bohm effect (AB effect). To experimentally confirm the effect, we set up an environment with $\boldsymbol{A}$ and ϕ, while zero electric field $\boldsymbol{E}$ and $\boldsymbol{B}$. Fig.1 shows an infinitely long solenoid placed by magnetic flux in the center, and an electric beam on both sides.

---Fig.1---

In a solenoid with radius r_0, enclose the magnetic flux Φ (flux is z-direction). The vector potential is given by:

$$\boldsymbol{A}(\boldsymbol{r}) = \begin{cases} (-\frac{y}{2\pi {r_0}^2}\Phi, \frac{x}{2\pi {r_0}^2}\Phi, 0) \ ; \ r_0 \geq r \geq 0 \\ (-\frac{y}{2\pi r^2}\Phi, \frac{x}{2\pi r^2}\Phi, 0) \ ; \ r \geq r_0 \end{cases} \tag{11a}$$

Where $(r = \sqrt{x^2 + y^2})$, the magnetic flux density $\boldsymbol{B} = \mathrm{rot}\boldsymbol{A}$ is given by:

$$\boldsymbol{B}(\boldsymbol{r}) = \begin{cases} (0, 0, \frac{\Phi}{2\pi {r_0}^2}) \ ; \ r_0 \geq r \geq 0 \\ (0, 0, 0) \ ; \ r \geq r_0 \end{cases} \tag{11b}$$

Hence, the magnetic flux cannot be produced outside the solenoid. In an environment where the wavefunction of an electron does not come inside the region of a solenoid, the vector potential $\boldsymbol{A}$ is directed toward tangent line (θ direction: $\tan\theta = x/y$) with its component actually becomes ($r > r_0$):

$$A_\theta = -\sin\theta A_x + \cos\theta A_y = \frac{\Phi}{2\pi r} = \nabla_\theta \frac{\Phi\theta}{2\pi} \tag{12}$$

$\nabla_\theta = (1/r)(\partial/\partial\theta)$ represents θ directional components of nabla ∇ by the polar display. The wavefunction at $\boldsymbol{A}=0$ we write ψ_0, and the wavefunction when $\boldsymbol{A}$ is in the phase (11), we write as ψ_Φ. The given $\boldsymbol{A}$ can be excluded by the gauge transformation $(\boldsymbol{A}'=0)$:

$$\boldsymbol{A} \to \boldsymbol{A} = \boldsymbol{A}' + \nabla\chi \ , \ \chi = \frac{\Phi}{2\pi}\arctan\frac{x}{y} = \frac{\Phi\theta}{2\pi} \tag{13}$$

So, we rewrite (10) with $\psi' = \psi_0, \psi = \psi_\Phi$:

$$\psi_\Phi = \psi_0 \exp(-\frac{ie\Phi\theta}{2\pi\hbar}) = \psi_0 \exp(-\frac{i\Phi\theta}{\phi_0}) \ ,$$
$$\phi_0 = \frac{h}{e} = 4.1 \times 10^{-15}\mathrm{Wb} \tag{14}$$

Accordingly, the Fig.1 shows that an electron traveling on the solenoid has progress in phase (magnetic flux is assumed to be facing towards the other side), while an electron traveling under the solenoid has delayed in phase. An interference pattern, which corresponds to the magnetic flux, is observed if the electric beam is projected on the screen. As the strength of magnetic flux changes, we can observe a shift in the interference patterns, therefore, an electron is found affected by the vector potential.

AB effect is demonstrated experimentally in the vacuum electric interference, however, by recent experiments, the similar interference of electric waves are observed in the metal. With a measurement of high quality conductor $1\mu\mathrm{m}$ or smaller, inelastic scattering of an electron hardly takes place below the absolute temperature $1\mathrm{K}$, hence the symmetry of wavefunction cannot be broken. Under such situation, create a loop to run an electric current in the electromagnetic field, which perpendicular to the loop. Then measure the electrical resistance as strength of the electric field continually makes changes. The resistance is observed to be fluctuating with the interval $\phi_0 = h/e$ of a function in terms of the strength of the magnetic flux. This also shows the occurrence of phase differences that arises the interference by an electron traveling around counterclockwise and the electron moving toward opposite direction in the loop because of the electric field.