Gauge transformation in quantum mechanics; Aharonov-Bohm effect

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David Joseph Bohm (20 December 1917 – 27 October 1992) was an American-born British quantum physicist who made contributions in the fields of theoretical physics, philosophy and neuropsychology, and to the Manhattan Project.

http://en.wikipedia.org/wiki/David_Bohm

Yakir Aharonov (born 1932 in Haifa, Israel) is an Israeli physicist specializing in Quantum Physics. He is a Professor of Theoretical Physics and the James J. Farley Professor of Natural Philosophy at Chapman University in California. He is also a distinguished professor in Perimeter Institute. He also serves as a professor emeritus at Tel Aviv University in Israel. He is president of the Iyar, The Israeli Institute for Advanced Research. His research interests are nonlocal and topological effects in quantum mechanics, quantum field theories and interpretations of quantum mechanics. In 1959, he and David Bohm proposed the Aharonov-Bohm Effect for which he co-received the 1998 Wolf Prize.

http://en.wikipedia.org/wiki/Yakir_Aharonov

Gauge transformation
Aharonov-Bohm effect
Young's double slits experiment
Vector potential

1. Gauge transformations in electromagnetism

We start with the Maxwell's equations,

$$\begin{cases} \nabla \cdot \boldsymbol{E} = 4\pi\rho \\ \nabla \times \boldsymbol{E} = -\dfrac{1}{c}\dfrac{\partial \boldsymbol{B}}{\partial t} \\ \nabla \cdot \boldsymbol{B} = 0 \\ \nabla \times \boldsymbol{B} = \dfrac{4\pi}{c}\boldsymbol{j} + \dfrac{1}{c}\dfrac{\partial \boldsymbol{E}}{\partial t} \end{cases}$$

where

B: magnetic field
E: electric field
ρ: charge density
J: current density

The Lorentz force is defined as

$$\boldsymbol{F} = q[\boldsymbol{E} + \frac{1}{c}(\boldsymbol{v} \times \boldsymbol{B})].$$

The Lorentz force is expressed in terms of fields ***E*** and ***B***, which is invariant under the gauge transformation (gauge independent). The magnetic field ***B*** and electric field ***E*** can be expressed by

$$\boldsymbol{B} = \nabla \times \boldsymbol{A},$$

$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} - \nabla\phi,$$

where ***A*** is a vector potential and ϕ is a scalar potential. When ***E*** and ***B*** are given, ϕ and ***A*** are not uniquely determined. If we have a set of possible values for the vector potential ***A*** and the scalar potential ϕ, we obtain other potentials ***A***' and ϕ' which describes the same electromagnetic field by the gauge transformation,

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi,$$

$$\phi' = \phi - \frac{1}{c}\frac{\partial \chi}{\partial t},$$

where χ is an arbitrary function of $\boldsymbol{r}$. We note that $\boldsymbol{B}$ and $\boldsymbol{E}$ are gauge-invariant;

$$\boldsymbol{B}' = \nabla \times \boldsymbol{A}' = \nabla \times (\boldsymbol{A} + \nabla \chi) = \nabla \times \boldsymbol{A} = \boldsymbol{B}$$

$$\boldsymbol{E}' = -\frac{1}{c}\frac{\partial \boldsymbol{A}'}{\partial t} - \nabla \phi' = -\frac{1}{c}\frac{\partial (\boldsymbol{A} + \nabla \chi)}{\partial t} - \nabla(\phi - \frac{1}{c}\frac{\partial \chi}{\partial t}) = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} - \nabla \phi = \boldsymbol{E}$$

2 Canonical momentum and mechanical momentum

We now consider the Lagrangian which is defined by

$$L = \frac{1}{2} m \boldsymbol{v}^2 - q(\phi - \frac{1}{c}\boldsymbol{v} \cdot \boldsymbol{A}),$$

where m and q are the mass and charge of the particle. The canonical momentum is defined as

$$\boldsymbol{p} = \frac{\partial L}{\partial \boldsymbol{v}} = m\boldsymbol{v} + \frac{q}{c}\boldsymbol{A}.$$

The mechanical momentum $\boldsymbol{\pi}$ is given by

$$\boldsymbol{\pi} = m\boldsymbol{v} = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}.$$

Then the Hamiltonian is obtained as

$$H = \boldsymbol{p} \cdot \boldsymbol{v} - L = (m\boldsymbol{v} + \frac{q}{c}\boldsymbol{A}) \cdot \boldsymbol{v} - L = \frac{1}{2} m \boldsymbol{v}^2 + q\phi = \frac{1}{2m}(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2 + q\phi.$$

The Hamiltonian formalism uses $\boldsymbol{A}$ and ϕ, and not $\boldsymbol{E}$ and $\boldsymbol{B}$, directly. The result is that the description of the particle depends on the gauge chosen.

3. Change of the wave function under a gauge transformation (by Mathematica)

The Schödinger equation contains the vector potential $\boldsymbol{A}$. It may imply that the wave function may change as the vector potential $\boldsymbol{A}$ and scalar potential ϕ is changed according to the gauge transformation,

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla \chi, \qquad \phi' = \phi - \frac{1}{c}\frac{\partial}{\partial t}\chi$$

The Schrödinger equation in the gauge ($\boldsymbol{A}$, ϕ) takes the form

$$[\frac{1}{2m}(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A})^2 - e\phi]\psi = i\hbar\frac{\partial}{\partial t}\psi \ .$$

where ψ, $\boldsymbol{A}$ and ϕ depends on $\boldsymbol{r}$ and t. We note that the charge of electron is denoted as $q=-e$ ($e>0$)
The Schrödinger equation in another gauge ($\boldsymbol{A}'$, ϕ') takes the form

$$[\frac{1}{2m}(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}')^2 - e\phi']\psi' = i\hbar\frac{\partial}{\partial t}\psi'$$

where ψ', $\boldsymbol{A}'$ and ϕ' depends on $\boldsymbol{r}$ and t. The wave function changes as

$$\psi' = \exp(-\frac{ie}{\hbar c}\chi)\psi ,$$

under the gauge transformation. The difference between ψ' and ψ is only the phase factor.

We now give a proof for this by using the Mathematica. We show that

$$[\frac{1}{2m}(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}+\frac{e}{c}\nabla\chi)^2 - e\phi + \frac{e}{c}\frac{\partial}{\partial t}\chi]\exp(-i\alpha\chi)\psi = i\hbar\frac{\partial}{\partial t}\exp(-i\alpha\chi)\psi$$

is equivalent to

$$[\frac{1}{2m}(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A})^2 - e\phi]\psi = i\hbar\frac{\partial}{\partial t}\psi \ .$$

First we assume that

$$\psi' = \exp(-i\alpha\chi)\psi$$

where α is just a parameter to be determined. We will show that

$$\alpha = \frac{e}{\hbar c} .$$

((**Mathematica**))
We assume that the electron charge is denoted by $-e_1$ in the program, which means $e_1>0$.
(i) We need to calculate directly

$$eq1 = [\frac{1}{2m}(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}+\frac{e}{c}\nabla\chi)^2 - e\phi + \frac{e}{c}\frac{\partial}{\partial t}\chi]\exp(-i\alpha\chi)\psi - i\hbar\frac{\partial}{\partial t}\exp(-i\alpha\chi)\psi$$

in the Cartesian co-ordinates. This equation reduces to

$$eq2 = \exp(-i\alpha\chi)\{[\frac{1}{2m}(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A})^2 - e\phi]\psi - i\hbar\frac{\partial}{\partial t}\psi\}$$

with $\alpha = \dfrac{e}{\hbar c}$.

The calculation without Mathematica is too complicated for me.

((**Program**))

Here is a Mathematica program which I made.

```
Clear["Global`*"]; χ1 = χ[x, y, z, t]; ex = {1, 0, 0};
ey = {0, 1, 0}; ez = {0, 0, 1}; Φ1 = Φ[x, y, z, t] - 1/c D[χ1, t];
ψ1 = ψ[x, y, z, t]; p := ħ/ⅈ Grad[#, {x, y, z}] &;
A1 = {Ax[x, y, z, t], Ay[x, y, z, t], Az[x, y, z, t]} +
  Grad[χ1, {x, y, z}]; Π1x := ex.(p[#] + e1/c A1 #) &;
Π1y := ey.(p[#] + e1/c A1 #) &; Π1z := ez.(p[#] + e1/c A1 #) &;
H1 :=
 (1/(2 m) (Π1x[Π1x[#]] + Π1y[Π1y[#]] + Π1z[Π1z[#]]) - e1 Φ1 #) &;

s1 = H1[ψ1] - ⅈ ħ D[ψ1, t] // FullSimplify;

rule1 =
  {ψ → (ψ0[#1, #2, #3, #4] Exp[- ⅈ α χ[#1, #2, #3, #4]] &)};
rule2 = {χ → 0, ψ → (ψ0[#1, #2, #3, #4] &)};

s2 = s1 //. rule1 // FullSimplify;
```

```
s3 = s1 /. rule2 // FullSimplify;

eq1 = ⅇ^(ⅈ α χ[x,y,z,t]) s2 - s3 // FullSimplify;

eq2 = Solve[eq1 == 0, α][[1]]
```

$\left\{\alpha \to \frac{\text{e1}}{c\,\hbar}\right\}$

```
(ⅇ^(ⅈ α χ[x,y,z,t]) s2)/s3 /. eq2 // FullSimplify
```

1

```
s3
```

$$-\frac{1}{2 c^2 m}\Big(-\text{e1}^2\,\text{Ax}[x,y,z,t]^2\,\psi0[x,y,z,t] - \text{e1}^2\,\text{Ay}[x,y,z,t]^2\,\psi0[x,y,z,t] - \text{e1}^2\,\text{Az}[x,y,z,t]^2\,\psi0[x,y,z,t] + 2 c^2\,\text{e1}\,m\,\Phi[x,y,z,t]\,\psi0[x,y,z,t] + 2 i c^2 m \hbar\,\psi0^{(0,0,0,1)}[x,y,z,t] + i c\,\text{e1}\,\hbar\,\psi0[x,y,z,t]\,\text{Az}^{(0,0,1,0)}[x,y,z,t] + 2 i c\,\text{e1}\,\hbar\,\text{Az}[x,y,z,t]\,\psi0^{(0,0,1,0)}[x,y,z,t] + c^2\hbar^2\,\psi0^{(0,0,2,0)}[x,y,z,t] + i c\,\text{e1}\,\hbar\,\psi0[x,y,z,t]\,\text{Ay}^{(0,1,0,0)}[x,y,z,t] + 2 i c\,\text{e1}\,\hbar\,\text{Ay}[x,y,z,t]\,\psi0^{(0,1,0,0)}[x,y,z,t] + c^2\hbar^2\,\psi0^{(0,2,0,0)}[x,y,z,t] + i c\,\text{e1}\,\hbar\,\psi0[x,y,z,t]\,\text{Ax}^{(1,0,0,0)}[x,y,z,t] + 2 i c\,\text{e1}\,\hbar\,\text{Ax}[x,y,z,t]\,\psi0^{(1,0,0,0)}[x,y,z,t] + c^2\hbar^2\,\psi0^{(2,0,0,0)}[x,y,z,t]\Big)$$

4 Analogy from Classical mechanics

The Newton's second law indicates that the position and the velocity take on, at every point, values independent of the gauge. Consequently,

$$\boldsymbol{r}' = \boldsymbol{r} \quad \text{and} \quad \boldsymbol{v}' = \boldsymbol{v},$$

or

$$\boldsymbol{\pi}' = \boldsymbol{\pi},$$

Since $\boldsymbol{\pi} = m\boldsymbol{v} = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}$, we have

$$\boldsymbol{p}' - \frac{q}{c}\boldsymbol{A}' = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}, \qquad \text{(Gauge independent)}$$

or

$$\boldsymbol{p}' = \boldsymbol{p} + \frac{q}{c}(\boldsymbol{A}' - \boldsymbol{A}) = \boldsymbol{p} + \frac{q}{c}\nabla\chi .$$

Note that q is the charge and $q = -e$ for the electron. In the Hamilton formalism, the value at each instant of the dynamical variables describing a given motion depends on the gauge chosen;

$$\langle\psi'|\hat{\boldsymbol{p}}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi|\psi\rangle.$$

5. Gauge invariance in quantum mechanics

In quantum mechanics, we describe the states in the old gauge and the new gauge as $|\psi\rangle$ and $|\psi'\rangle$. The analogue of the relation in the classical mechanics is thus given by the relations between average values.

$$\langle\psi'|\hat{\boldsymbol{r}}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{r}}|\psi\rangle \qquad \text{(gauge independent)}$$

$$\langle\psi'|\hat{\boldsymbol{p}}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi|\psi\rangle \qquad \text{(gauge independent)}$$

This can be rewritten as

$$\langle\psi'|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}'|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}|\psi\rangle .$$

This equivalence will be proved later.

We now seek a unitary operator $\hat{U}$ which enables one to go from $|\psi\rangle$ to $|\psi'\rangle$.

$$|\psi'\rangle = \hat{U}|\psi\rangle .$$

From the condition $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle$, we have

$$\hat{U}^{+}\hat{U} = \hat{U}\hat{U}^{+} = \hat{1}$$

From the condition, $\langle\psi'|\hat{\boldsymbol{r}}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{r}}|\psi\rangle$

$$\hat{U}^{+}\hat{\boldsymbol{r}}\hat{U} = \hat{\boldsymbol{r}},$$

or

$$[\hat{\boldsymbol{r}},\hat{U}] = 0 = i\hbar\frac{\partial \hat{U}}{\partial \hat{\boldsymbol{p}}}$$

$\hat{U}$ is independent of $\hat{\boldsymbol{p}}$. We also get

$$\hat{U}^{+}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}')\hat{U} = \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}$$

or

$$\hat{U}^{+}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A} - \frac{q}{c}\nabla\chi)\hat{U} = \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}$$

or

$$\begin{aligned}\hat{U}^{+}\hat{\boldsymbol{p}}\hat{U} &= \frac{q}{c}\hat{U}^{+}\boldsymbol{A}\hat{U} + \frac{q}{c}\hat{U}^{+}\nabla\chi\hat{U} + \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A} \\ &= \frac{q}{c}\boldsymbol{A} + \frac{q}{c}\nabla\chi + \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A} \\ &= \hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi\end{aligned}$$

Note that $[\hat{\boldsymbol{r}},\hat{U}] = 0$, and $\boldsymbol{A}$ is a function of $\hat{\boldsymbol{r}}$.

6. Proof of the expression $\langle\psi'|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}'|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}|\psi\rangle$

Here we show that

$$\langle\psi'|\hat{\boldsymbol{p}}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi|\psi\rangle$$

is equivalent to

$$\langle\psi'|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}'|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}|\psi\rangle,$$

where $\hat{\boldsymbol{\pi}} = \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}$ and $\boldsymbol{A}' = \boldsymbol{A} + \frac{q}{c}\nabla\chi$.

((**Proof**))

$$\langle\psi'|\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}'|\psi'\rangle = \langle\psi'|\hat{\boldsymbol{p}}|\psi'\rangle - \langle\psi'|\frac{q}{c}\boldsymbol{A}'|\psi'\rangle$$
$$= \langle\psi|\hat{\boldsymbol{p}}+\frac{q}{c}\nabla\chi|\psi\rangle - \langle\psi|\hat{U}^{+}\frac{q}{c}\boldsymbol{A}'\hat{U}|\psi\rangle$$
$$= \langle\psi|\hat{\boldsymbol{p}}+\frac{q}{c}\nabla\chi|\psi\rangle - \langle\psi|\hat{U}^{+}\hat{U}\frac{q}{c}\boldsymbol{A}'|\psi\rangle$$
$$= \langle\psi|\hat{\boldsymbol{p}}+\frac{q}{c}\nabla\chi|\psi\rangle - \langle\psi|\frac{q}{c}\boldsymbol{A}'|\psi\rangle$$
$$= \langle\psi|\hat{\boldsymbol{p}}+\frac{q}{c}\nabla\chi-\frac{q}{c}\boldsymbol{A}'|\psi\rangle$$
$$= \langle\psi|\hat{\boldsymbol{p}}-\frac{q}{c}(\boldsymbol{A}'-\nabla\chi)|\psi\rangle$$
$$= \langle\psi|\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}|\psi\rangle$$

where $[\hat{U},\boldsymbol{A}'] = \hat{0}$, since $\boldsymbol{A}'$ is a function of $\hat{\boldsymbol{r}}$.

Here we note that

$$\langle\psi'|\hat{U}^{+}(\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}')\hat{U}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}|\psi\rangle$$

leading to the relations

$$\hat{U}^{+}(\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}')\hat{U} = \hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A},$$

and

$$\hat{U}(\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A})\hat{U}^{+} = \hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}'.$$

7. Expression of the unitary operator

We assert that $\hat{U}$

$$\hat{U} = \exp[\frac{iq}{\hbar c}\chi(\hat{\boldsymbol{r}})], \qquad \hat{U}^{+} = \exp[-\frac{iq}{\hbar c}\chi(\hat{\boldsymbol{r}})].$$

Then we get

$$\hat{U}^+\hat{\boldsymbol{p}}\hat{U} = \hat{U}^+[\hat{\boldsymbol{p}},\hat{U}] + \hat{\boldsymbol{p}}$$
$$= -\hat{U}^+ i\hbar\frac{\partial}{\partial\hat{\boldsymbol{r}}}\hat{U} + \hat{\boldsymbol{p}}$$
$$= -\hat{U}^+\hat{U} i\hbar\frac{iq}{\hbar c}\nabla\chi + \hat{\boldsymbol{p}}$$
$$= \hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi$$

which coincides with the expression described above.

$$\langle\psi'|\hat{\boldsymbol{p}}|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi|\psi\rangle, \qquad \hat{U}^+\hat{\boldsymbol{p}}\hat{U} = \hat{\boldsymbol{p}} + \frac{q}{c}\nabla\chi$$

((Note)) We use the notation such that

$$\frac{\partial}{\partial\hat{\boldsymbol{r}}}\hat{U} = \frac{iq}{\hbar c}\hat{U}\frac{\partial\chi(\hat{\boldsymbol{r}})}{\partial\hat{\boldsymbol{r}}} = \frac{iq}{\hbar c}\hat{U}(\nabla\chi).$$

So we get the gauge transformation for the wave function;

$$|\psi'\rangle = \hat{U}|\psi\rangle = \exp[\frac{iq}{\hbar c}\chi(\hat{\boldsymbol{r}})]|\psi\rangle.$$

or

$$\langle\boldsymbol{r}|\psi'\rangle = \exp[\frac{iq}{\hbar c}\chi(\boldsymbol{r})]\langle\boldsymbol{r}|\psi\rangle$$

The phase factor of the wave function depends on the choice of the form of χ in the gauge transformation.

8. Hamiltonian under the gauge transformation

We consider the Schrödinger equation given by

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle.$$

and

$$i\hbar\frac{\partial}{\partial t}|\psi'\rangle = \hat{H}'|\psi'\rangle,$$

or

$$i\hbar\frac{\partial}{\partial t}\hat{U}|\psi\rangle = \hat{H}'\hat{U}|\psi\rangle,$$

or

$$i\hbar[\frac{\partial\hat{U}}{\partial t}|\psi\rangle + \hat{U}\frac{\partial}{\partial t}|\psi\rangle] = \hat{H}'\hat{U}|\psi\rangle.$$

Since $\frac{\partial\hat{U}}{\partial t} = \frac{iq}{\hbar c}\frac{\partial\chi}{\partial t}\hat{U}$, we get

$$-\frac{q}{c}\frac{\partial\chi}{\partial t}\hat{U}|\psi\rangle + \hat{U}i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}'\hat{U}|\psi\rangle,$$

or

$$-\frac{q}{c}\frac{\partial\chi}{\partial t}\hat{U}|\psi\rangle + \hat{U}\hat{H}|\psi\rangle = \hat{H}'\hat{U}|\psi\rangle,$$

or

$$\hat{H}'\hat{U} = -\frac{q}{c}\frac{\partial\chi}{\partial t}\hat{U} + \hat{U}\hat{H}.$$

Thus we have

$$\hat{H}' = -\frac{q}{c}\frac{\partial\chi}{\partial t} + \hat{U}\hat{H}\hat{U}^{+}.$$

We note that

$$\hat{U}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A})\hat{U}^{+} = (\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}'),$$

Then we have

$$\hat{U}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A})^{2}\hat{U}^{+} = \hat{U}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A})\hat{U}^{+}\hat{U}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A})\hat{U}^{+} = (\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}')^{2}$$

Using this relation we get the new Hamiltonian as

$$\hat{H}' = -\frac{q}{c}\frac{\partial\chi}{\partial t} + \hat{U}[\frac{1}{2m}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A})^{2} + q\phi]\hat{U}^{+}$$

or

$$\hat{H}' = -\frac{q}{c}\frac{\partial \chi}{\partial t} + \frac{1}{2m}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}')^2 + q\phi = \frac{1}{2m}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}')^2 + q\phi'.$$

Therefore the Schrödinger equation can be written in the same way in any gauge chosen.

9. Invariance of physical predictions under a gauge transformation

The current density is invariant under the gauge transformation. The current density is given by

$$\boldsymbol{J} = \frac{1}{m}\mathrm{Re}[\langle\psi|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}|\psi\rangle]$$

We note that

$$\langle\psi'|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}'|\psi'\rangle = \langle\psi|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}|\psi\rangle$$

Here we have

$$\hat{U}^+(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}')\hat{U} = \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}$$

Then

$$\boldsymbol{J}' = \frac{1}{m}\mathrm{Re}[\langle\psi'|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}'|\psi'\rangle] = \frac{1}{m}\mathrm{Re}[\langle\psi|\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}|\psi\rangle] = \boldsymbol{J}$$

Note: after the gauge transformation, $\boldsymbol{A} \rightarrow \boldsymbol{A}'$ in the current density operator. This is identified from the form of Hamiltonian.

$$\hat{H}' = \frac{1}{2m}(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}')^2 + q\phi'.$$

We note that the density is gauge invariant under the gauge transformation.

$$\rho' = |\langle\boldsymbol{r}|\psi'\rangle|^2 = \rho = |\langle\boldsymbol{r}|\psi\rangle|^2.$$

since

$$\hat{U} = \exp[\frac{iq}{\hbar c}\chi(\hat{\boldsymbol{r}})]$$

$$\langle \boldsymbol{r}|\psi'\rangle = \langle \boldsymbol{r}|\hat{U}(\boldsymbol{r})|\psi\rangle = \exp[\frac{iq}{\hbar c}\chi(\boldsymbol{r})]\langle \boldsymbol{r}|\psi\rangle$$

$$|\langle \boldsymbol{r}|\psi'\rangle| = \left|\exp[\frac{iq}{\hbar c}\chi(\boldsymbol{r})]\right|^2 |\langle \boldsymbol{r}|\psi\rangle|^2 = |\langle \boldsymbol{r}|\psi\rangle|^2$$

10. Aharonov-Bohm effect

In the best known version, electrons are aimed so as to pass through two regions that are free of electromagnetic field, but which are separated from each other by a long cylindrical solenoid (which contains magnetic field line), arriving at a detector screen behind. At no stage do the electrons encounter any non-zero field ***B***.

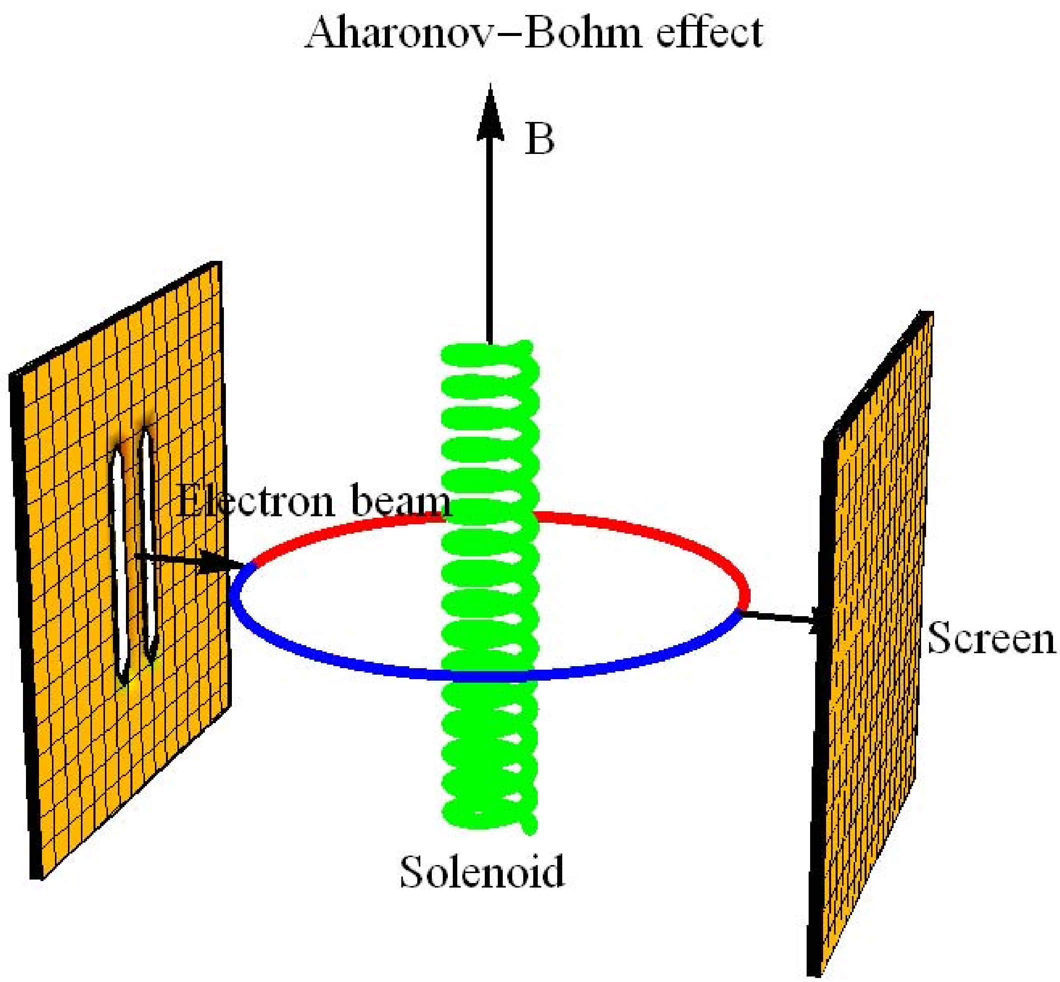

Fig. Schematic diagram of the Aharonov-Bohm experiment. Electron beams are split into two paths that go to either a collection of lines of magnetic flux (achieved by means of a long solenoid). The beams are brought together at a screen, and the resulting quantum interference pattern depends upon the magnetic flux strength- despite the fact that the electrons only encounter a zero magnetic field. Path denoted by red (counterclockwise). Path denoted by blue (clockwise)

We assume that $q = -e$ (e>0). In the space when $\boldsymbol{B} = 0$, we have

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} = 0 ,$$

or

$$\boldsymbol{A} = \nabla \chi ,$$

or

$$\chi(\boldsymbol{r}) = \int_{r_o}^{r} d\boldsymbol{r} \cdot \boldsymbol{A}(\boldsymbol{r}) ,$$

where $\boldsymbol{r}_0$ is an arbitrary initial point in the field region. We now consider the gauge transformation such that

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla(-\chi) = 0 .$$

The new wavefunction $\psi'(\mathbf{r})$ can be written as

$$\psi'(\boldsymbol{r}) = \exp(\frac{ie\chi}{\hbar c})\psi(\boldsymbol{r}) .$$

The Schrödinger equation for $\psi'(\mathbf{r})$ is

$$-\frac{\hbar^2}{2m}\nabla^2\psi' = i\hbar\frac{\partial}{\partial t}\psi' ,$$

where ψ' is the field-free wave function and the new Hamiltonian is that of free particle;

$$\hat{H}' = \frac{1}{2m}\hat{\boldsymbol{p}}^2 .$$

Then we have

$$\psi = \psi' \exp(-\frac{ie\chi}{\hbar c}) = \psi' \exp[-\frac{ie}{\hbar c}\int_{r_o}^{r} d\boldsymbol{r} \cdot \boldsymbol{A}(\boldsymbol{r})] ,$$

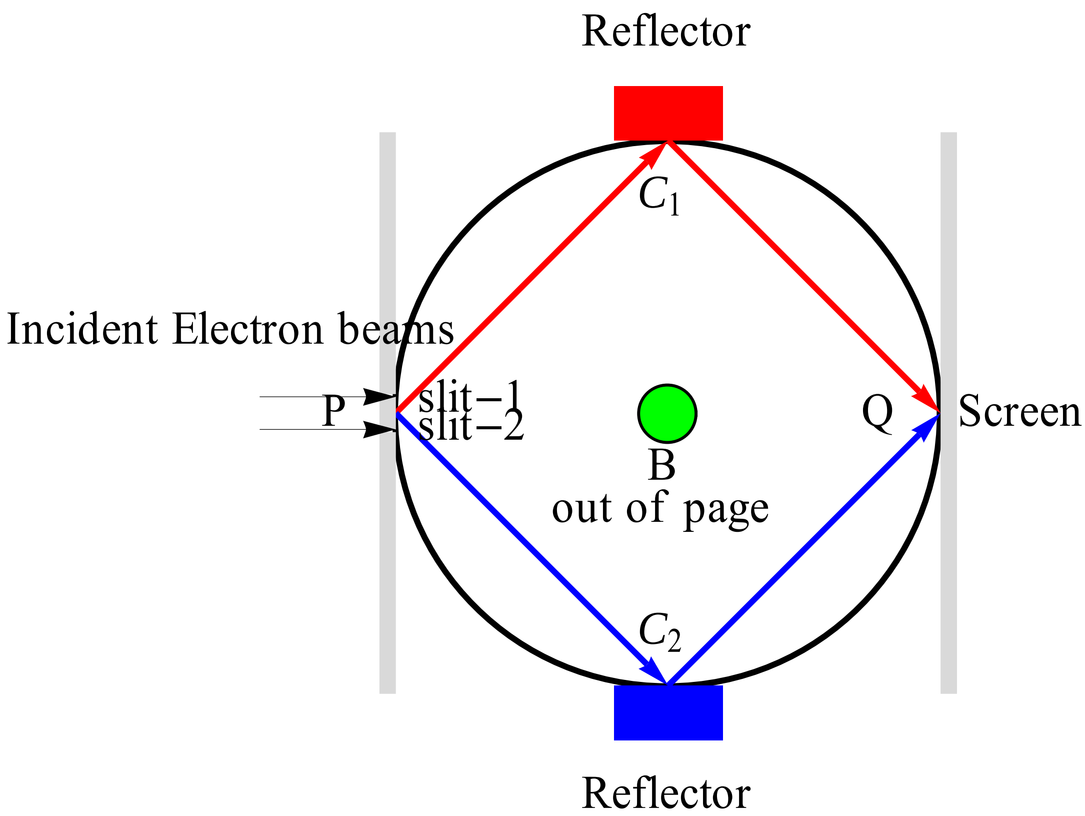

Fig. Schematic diagram of the Aharonov-Bohm experiment. Incident electron beams go into the two narrow slits (one beam denoted by blue arrow, and the other beam denoted by red arrow). The diffraction pattern is observed on the screen. The reflector plays a role of mirror for the optical experiment.

Let ψ_{1B} be the wave function when only slit 1 is open.

$$\psi_{1,B}(\boldsymbol{r}) = \psi_{1,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path1} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})], \tag{1}$$

The line integral runs from the source through slit 1 to $\boldsymbol{r}$ (screen). Similarly, for the wave function when only slit 2 is open, we have

$$\psi_{2,B}(\boldsymbol{r}) = \psi_{2,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})], \tag{2}$$

The line integral runs from the source through slit 2 to $\boldsymbol{r}$ (screen). Superimposing Eqs.(1) and (2), we obtain

$$\psi_{B}(\boldsymbol{r}) = \psi_{1,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path1} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})] + \psi_{2,0}(\boldsymbol{r})\exp[-\frac{ie}{\hbar c}\int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})]$$

The relative phase of the two terms is

$$\int_{Path1} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) - \int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) = \oint d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r}) = \int d\boldsymbol{a}\cdot(\nabla\times\boldsymbol{A})$$
$$= \int d\boldsymbol{a}\cdot\boldsymbol{B} = \Phi_B$$

by using the Stokes' theorem. Φ_B is the magnetic flux. Then we have

$$\psi_B(\boldsymbol{r}) = \exp[-\frac{ie}{\hbar c}\int_{Path2} d\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{r})][\psi_{1,0}(\boldsymbol{r})\exp(-\frac{ie}{\hbar c}\Phi_B) + \psi_{2,0}(\boldsymbol{r})],$$

where the relative phase now is expressed in terms of the flux of the magnetic field through the closed path.

When

$$\frac{e}{\hbar c}\Phi_B = \frac{e}{\hbar c}\int_{\substack{Closed\\path}} d\boldsymbol{a}\cdot\boldsymbol{B} = 2\pi n \quad (n = 0, 1, 2, 3,\ldots).$$

The pattern will be the same as without the magnetic field present.

When

$$\frac{e}{\hbar c}\Phi_B = \frac{e}{\hbar c}\int_{\substack{Closed\\path}} d\boldsymbol{a}\cdot\boldsymbol{B} = 2\pi(n+\frac{1}{2}),$$

or

$$\Phi_B = \frac{2\pi\hbar c}{e}(n+\frac{1}{2}) = 2\Phi_0(n+\frac{1}{2}),$$

the position of the minimum and the maximum in the pattern will be interchanged. Φ_0 is the magnetic flux quanta and is given by

$$\Phi_0 = \frac{2\pi\hbar c}{2e} = \frac{hc}{2e} = 2.067833667 \text{ x } 10^{-7} \text{ Gauss cm}^2 = 2.067833667 \text{ x } 10^{-15} \text{ T m}^2.$$

((**Note**))

$$\psi_{1,0}(\mathbf{r}) \approx e^{ikr_1}, \qquad \psi_{2,0}(\mathbf{r}) \approx e^{ikr_2}$$

The condition for constructive interference in the presence of a magnetic field is

$$kr_1 - \frac{e}{\hbar c}\Phi_B - kr_2 = 2\pi\ell$$

where *l* is intergers.

$$r_1 - r_2 = \frac{1}{k}(\frac{e}{\hbar c}\Phi_B + 2\pi\ell).$$

The positions of the interference maxima are shifted due to the variation in Φ_B, although the electron does not penetrate into the region of finite magnetic field.

(i) When $\frac{e}{\hbar c}\Phi_B = 2\pi n$

$$r_1 - r_2 = \frac{1}{k}2\pi(n + \ell).$$

The pattern is the same as without *B*.

(ii) When $\frac{e}{\hbar c}\Phi_B = 2\pi(n + \frac{1}{2})$,

$$r_1 - r_2 = \frac{1}{k}2\pi(n + \ell + \frac{1}{2}).$$

The pattern is different from that without *B*.

11. Young's double slit experiment for the Aharonov-Bohm effect

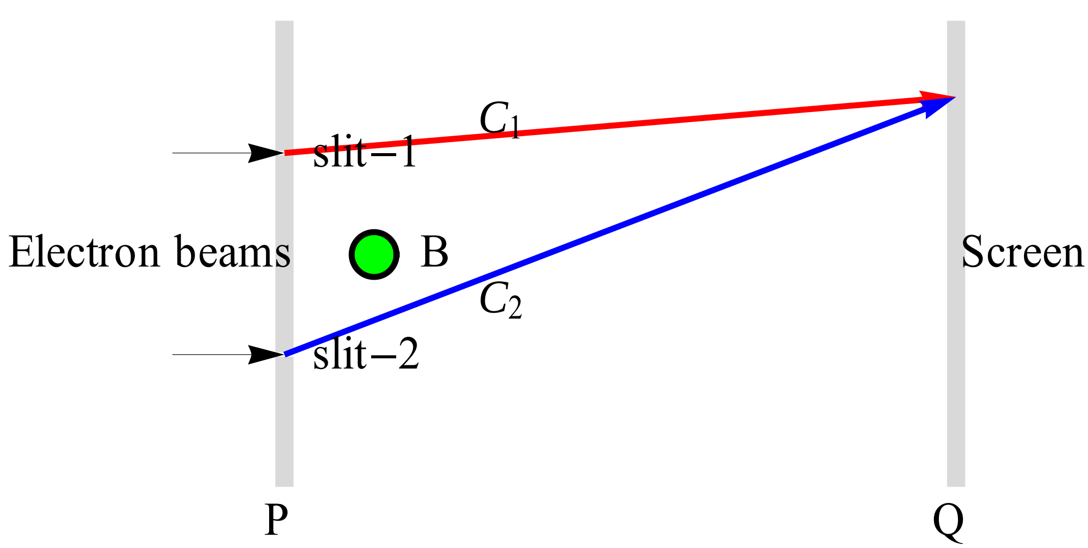

Fig. Young's double slit experiment with the electron beam source. The magnetic field is applied just behind the slits. There is no magnetic field around the paths (C_1 and C_2).

$$\phi_B = \frac{e}{\hbar c}\Phi_B = \frac{eBA}{\hbar c}.$$

$$\left|r_2 - r\right|_1 = d\sin\theta.$$

The phase difference;

$$\phi_0 = \frac{2\pi}{\lambda}\left|r_2 - r_1\right| = \frac{2\pi}{\lambda}d\sin\theta \approx \frac{2\pi}{\lambda}d\theta$$

Since $y = D\tan\theta \approx D\theta$, we have

$$\phi_0 = \frac{2\pi}{\lambda}\frac{d}{D}y.$$

The intensity I

$$I = \left|\psi_B(\mathbf{r})\right|^2 = [1 + e^{i(\phi_0 - \phi_B)}][1 + e^{-i(\phi_0 - \phi_B)}] = 4\sin^2(\frac{\phi_0 - \phi_B}{2}).$$

The intensity is described by

$$I = 4\sin^2(\frac{\phi_0 - \phi_B}{2}) = 4\sin^2(\frac{\frac{2\pi}{\lambda}\frac{d}{D}y - \frac{eBA}{\hbar c}}{2}).$$

When the effect of the width of the slit a is taken into account, the intensity is modified as

$$I = 4\sin^2(\frac{\phi_0 - \phi_B}{2}) = 4\sin^2(\frac{\frac{2\pi}{\lambda}\frac{d}{D}y - \frac{eBA}{\hbar c}}{2})\frac{\sin^2\beta}{\beta^2},$$

where

$$\beta = \frac{\pi a}{\lambda}\sin\theta \approx \frac{\pi a}{\lambda}\theta = \frac{\pi a}{\lambda}\frac{y}{D}.$$

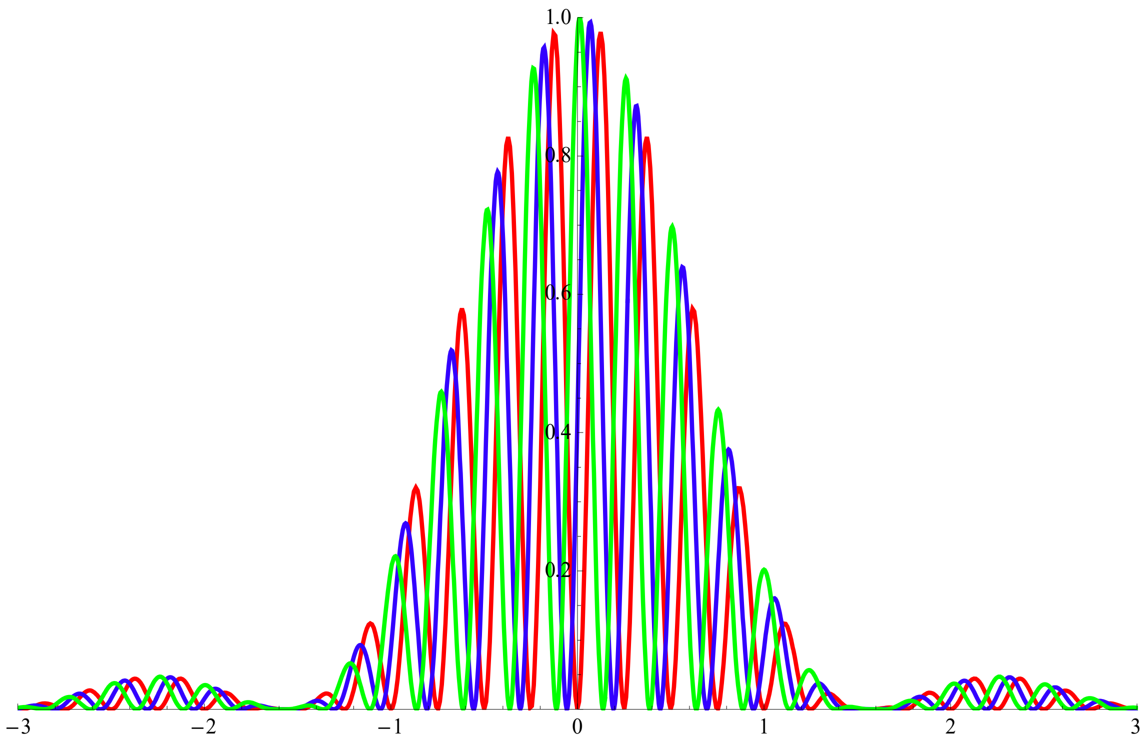

Fig. Young's double slits diffraction with Aharonov-Bohm effect. The diffraction pattern changes with the magnetic field. red (B = 0). Blue (B=intermediate value). Green (B = stronger field).

12. The observation of Aharonov-Bohm effect by Akira Tonomura

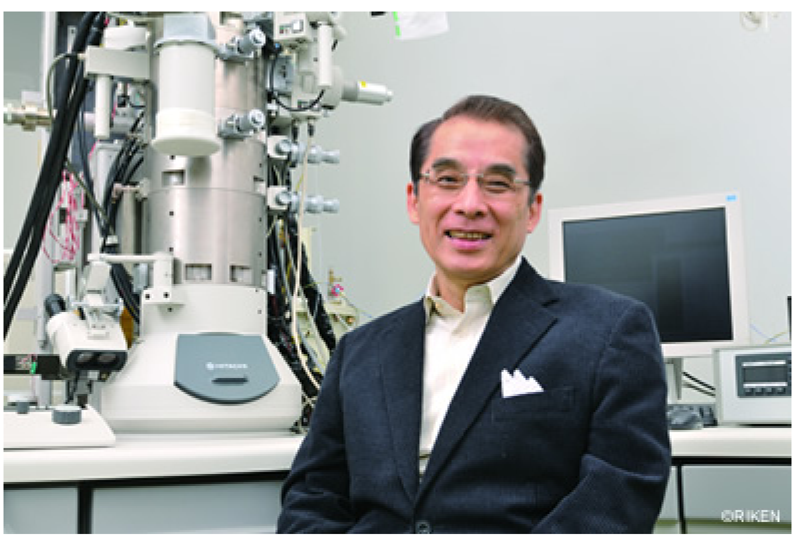

Fig. Picture of Dr Akira Tonomura (April 25, 1942– May 2, 2012), who was a Japanese physicist, best known for his development of electron holography and his experimental verification of the Aharonov–Bohm effect. http://en.wikipedia.org/wiki/Akira_Tonomura

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Summary of the article (by A. Tonomura)
[http://physicaplus.org.il/zope/home/en/1224031001/Tonomura_en]

(i) A toroidal ferromagnet (permalloy) instead of a straight solenoid, which has inevitable leakage fluxes from both ends of the solenoid. An ideal geometry with no flux leakage can be achieved by the finite system of a toroidal magnetic field.

(ii) The toroidal ferromagnet is covered with a superconducting niobium layer to completely confine the magnetic field.

(iii) An electron wave is incident to a tiny toroidal sample fabricated using lithography techniques.

(iv) The relative phase shift between two waves passing through the hole and around the toroid is measured as an interferogram. A relative phase shift of π is produced, indicating the existence of the AB effect even when the magnetic fields are confined within the superconductor and shielded from the electron wave. An electron wave must be physically influenced by the vector potentials. Therefore, it can be concluded that electron waves passing through the field-free regions inside and outside the toroidal magnet are phase-shifted by π, although the waves never touch the magnetic fields.

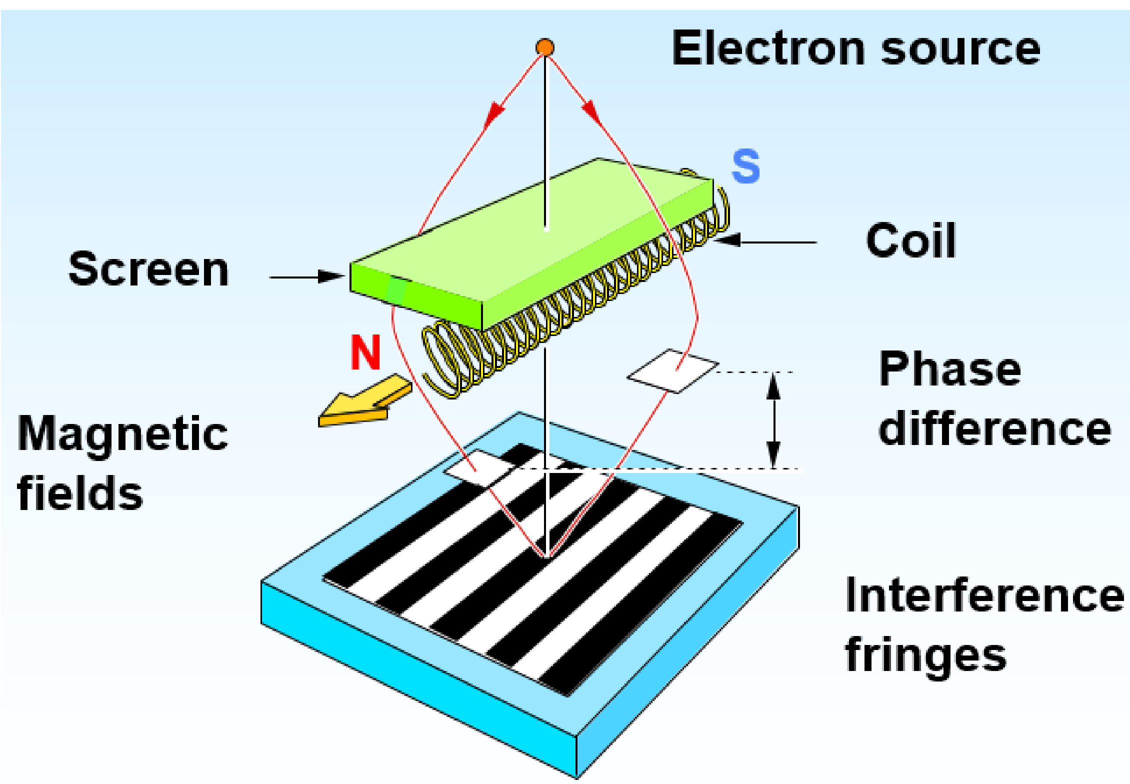


Fig. Schematic diagram of the Aharonov-Bohm effect (by A. Tonomura group at Hitachi).

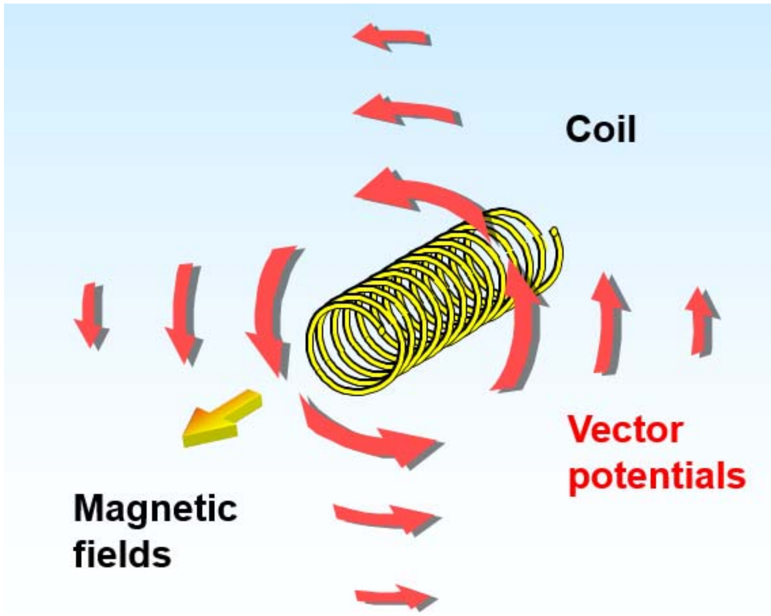


Fig. The direction of the vector potential around the solenoid coil.

Vector potential around the solenoid

$$\Phi = \int \boldsymbol{B} \cdot d\boldsymbol{a} = \int (\nabla \times \boldsymbol{A}) \cdot d\boldsymbol{a} = \oint \boldsymbol{A} \cdot d\boldsymbol{l}$$

Then we have

$$A_\phi 2\pi r = \Phi , \qquad \text{or} \qquad A_\phi = \frac{\Phi}{2\pi r}$$

where the vector potential *A* is in a two dimensional plane perpendicular to the axis of solenoid. $\boldsymbol{A} = A_\theta \boldsymbol{e}_\theta$. $\boldsymbol{e}_\theta$ is the unit vector along the tangential direction.

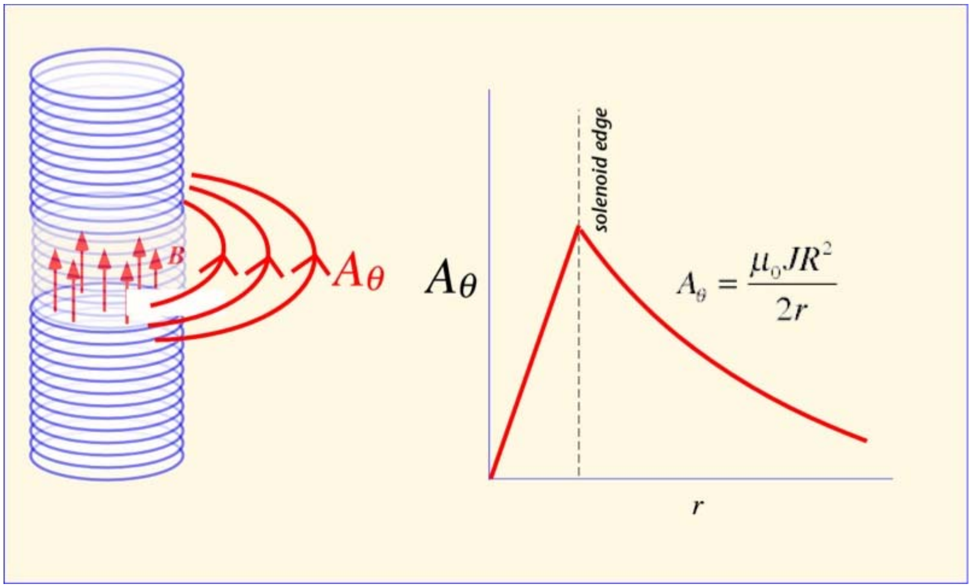
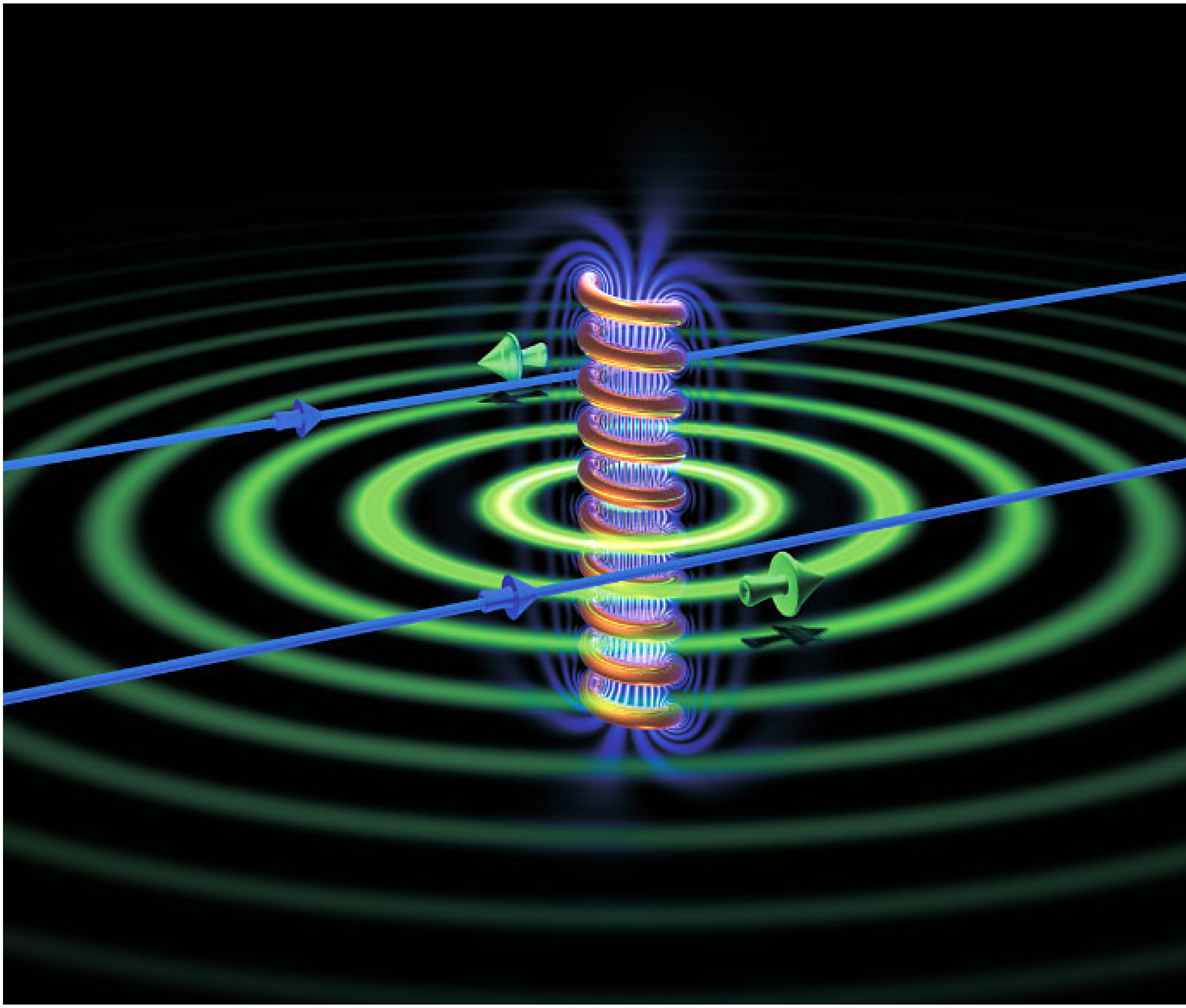


Fig. The vector potential distribution around the solenoid.



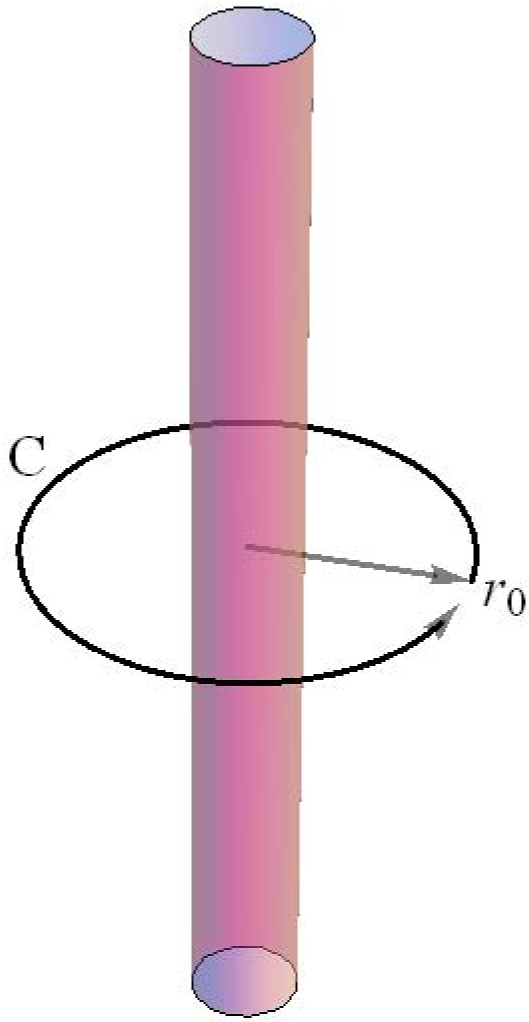
http://prlo.aps.org/files/focus/v28/st4/ABeffect_BIG.jpg

Look Ma, no fields. Electrons passing around opposite sides of an electromagnet feel negligible magnetic fields (purple), but the electromagnetic potential (green circles and arrows) affects them in opposite ways, leading to measurable consequences. Before the effect was proposed in 1959, physicists thought fields must interact directly with particles to cause measurable electromagnetic effects.

13. Flux quantization in superconductors

The electrons form a Cooper pairs in superconductors. The wavefunction of the Cooper pairs in the absence of a field is given by $\psi_0(\boldsymbol{r})$. Then in a presence of a field, it becomes

$$\psi_B(\boldsymbol{r}) = \exp[-\frac{2ie}{\hbar c}\int_{r_0}^{r} d\boldsymbol{s}\cdot \boldsymbol{A}(\boldsymbol{s})]\psi_0(\boldsymbol{r})$$



A closed path (C) about the cylinder starting at the point r_0 gives

$$\psi_B(\boldsymbol{r}_0) = \psi_0(\boldsymbol{r}) = \exp[-\frac{2ie}{\hbar c}\int_C d\boldsymbol{s}\cdot \boldsymbol{A}]\psi_0(\boldsymbol{r}_0)$$

Since the wavefunction should be single valued, we must have

$$\exp[-\frac{2ie}{\hbar c}\int_C d\boldsymbol{s}\cdot\boldsymbol{A}]=1$$

or

$$\frac{2e}{\hbar c}\int_C d\boldsymbol{s}\cdot\boldsymbol{A}=2n\pi$$

or

$$\Phi_B=\int_C d\boldsymbol{s}\cdot\boldsymbol{A}=\frac{2n\pi\hbar c}{2e}=n\frac{hc}{2e}$$

where we use the Stokes theorem,

$$\int_C d\boldsymbol{s}\cdot\boldsymbol{A}=\int_A d\boldsymbol{a}\cdot\nabla\times\boldsymbol{A}=\int_A d\boldsymbol{a}\cdot B=\Phi_B$$

where Φ_B is the total magnetic flux. Then quantized magnetic flux is given by

$$\Phi_0=\frac{2\pi c\hbar}{2e}=\frac{hc}{2e}=2.06783372\times10^{-7}\text{ Gauss cm}^2$$

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Mathematica demonstration
http://demonstrations.wolfram.com/AharonovBohmEffect/

APPENDIX-I
Magnetic field distribution

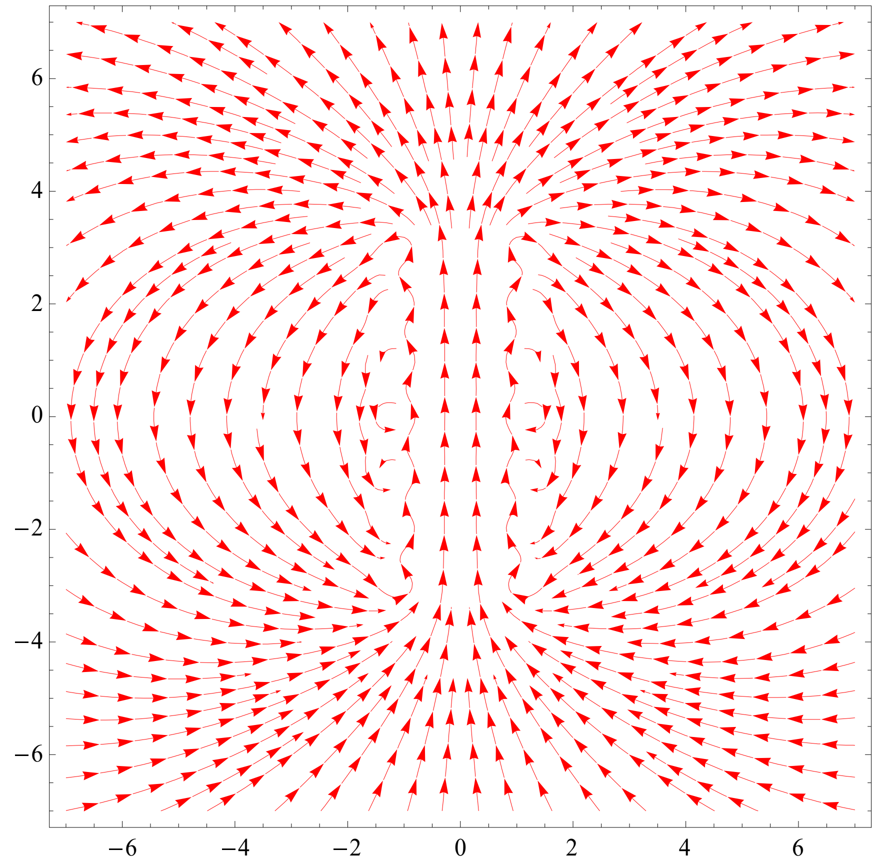
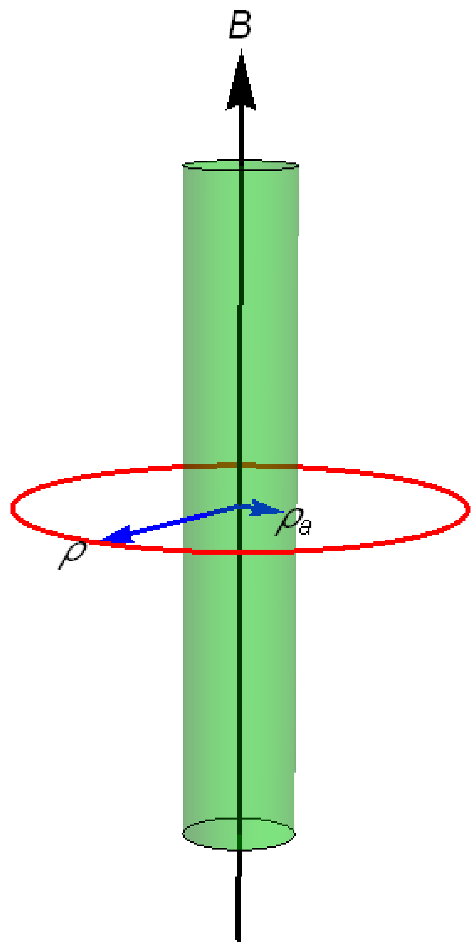


Fig. Magnetic field lines of the system of 7 current loops stacked along the z axis, which are equally spaced. When the coil is wound tightly and there are more loops, the magnetic field inside become larger and more uniform. The magnetic field $\boldsymbol{B}$ forms a closed loop.

APPENDIX-II
Aharonov-Bohm effect
The property of the wave function around the cylinder in which an external magnetic field is applied. (Sakurai and Napolitano)

We consider a hollow cylindrical shell, as shown in the above figure. We assume that an electron of charge ($-e$) can be completely confined to the interior of the shell with rigid walls. The wave function is required to vanish on the inner ($\rho = \rho_a$) and outer ($\rho = \rho_b$) walls, as well as at the top and bottom. It is a straightforward boundary value problem in mathematical physics to obtain the energy eigenvalues.



We consider a very long solenoid into the hole in the middle in such a way that no magnetic field leaks into the region $\rho \geq \rho_a$. The boundary conditions for the wave function are taken to be the same as before; the walls are assumed to be just as rigid. Intuitively, we may conjecture that the energy spectrum is unchanged because the region with $B \neq 0$ is completely inaccessible to the charged particle trapped inside the shell. However, quantum mechanics tells us that this conjecture is not correct.

Even though the magnetic field vanishes in the interior, the vector potential $\boldsymbol{A}$ is nonvanishing there; using Stokes's theorem, we can infer that the vector potential needed to produce the magnetic field B (= B_z) is

$$\Phi = \int \boldsymbol{B} \cdot d\boldsymbol{a} = \int (\nabla \times \boldsymbol{A}) \cdot d\boldsymbol{a} = \int \boldsymbol{A} \cdot d\boldsymbol{r} = A_\phi (2\pi\rho)$$

or

$$A_\phi = \frac{\Phi}{2\pi\rho} = \frac{\Phi_a}{2\pi\rho} = \frac{B\pi\rho_a^{\ 2}}{2\pi\rho} = \frac{B\rho_a^{\ 2}}{2\rho} \qquad \text{for} \qquad \rho \geq \rho_a$$

where Φ_a is the total magnetic flux penetrating the cylinder along the *z* axis,

$$\Phi_a = B\pi\rho_a^{\ 2}.$$

We now consider the gauge transformation such that

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi = 0.$$

Since

$$\nabla\chi = \boldsymbol{e}_\rho \frac{\partial\chi}{\partial\rho} + \boldsymbol{e}_z \frac{\partial\chi}{\partial z} + \boldsymbol{e}_\phi \frac{1}{\rho}\frac{\partial\chi}{\partial\phi}$$

we get

$$A_\phi + \frac{1}{\rho}\frac{\partial\chi}{\partial\phi} = 0.$$

Then we have

$$\frac{B\rho_a^{\ 2}}{2\rho} + \frac{1}{\rho}\frac{\partial\chi}{\partial\phi} = 0, \qquad \frac{\partial\chi}{\partial\phi} + \frac{\Phi_a}{2\pi} = 0,$$

or

$$\chi = -\frac{\Phi_a}{2\pi}\phi.$$

The wave function (ψ')for the free particle satisfies the Schrődinger equation (free particle) is given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi' = E_k\psi' = \frac{\hbar^2}{2m}k^2\psi'$$

where

$$E_k = \frac{\hbar^2}{2m}k^2$$

Noting that

$$\nabla^2\psi' = \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\psi'}{\partial\rho}) + \frac{1}{\rho^2}\frac{\partial^2\psi'}{\partial\phi^2} + \frac{\partial^2\psi'}{\partial z^2}$$

When ψ' depends only on ϕ (ρ is kept as fixed parameter), we have

$$-\frac{\hbar^2}{2m}\frac{1}{\rho^2}\frac{\partial^2\psi'}{\partial\phi^2} = \frac{\hbar^2}{2m}k^2\psi'$$

or

$$\frac{\partial^2\psi'}{\partial\phi^2} + k^2\rho^2\psi' = 0$$

The solution of this equation is

$$\psi' = \psi_0 e^{ik\rho\phi}$$

Using the gauge transformation of the wave function, we get

$$\psi' = \psi \exp(-\frac{ie}{\hbar c}\chi)$$

or

$$\begin{aligned}
\psi &= \psi' \exp(\frac{ie}{\hbar c}\chi) \\
&= \psi_0 \exp(ik\rho\phi)\exp(-\frac{ie}{\hbar c}\frac{\Phi_a}{2\pi}\phi) \\
&= \psi_0 \exp(ik\rho\phi)\exp(-i\frac{\Phi_a}{2\Phi_0}\phi) \\
&= \psi_0 \exp[i(k\rho - \frac{\Phi_a}{2\Phi_0})\phi]
\end{aligned}$$

where

$$\chi = -\frac{\Phi_a}{2\pi}\phi, \qquad \Phi_0 = \frac{hc}{2e} = \frac{\pi\hbar c}{e} \qquad \text{(quantum magnetic flux, fluxoide)}$$

We use the boundary condition such that

$$\psi(\phi + 2\pi) = \psi(\phi)$$

or

$$\exp[i2\pi(k\rho - \frac{\Phi_a}{2\Phi_0})] = 1$$

or

$$2\pi(k\rho - \frac{\Phi_a}{2\Phi_0}) = 2\pi(-n)$$

where n is an integer; $n = 0, \pm1, \pm2, \ldots.$

$$k = \frac{1}{\rho}\left(\frac{\Phi_a}{2\Phi_0} - n\right)$$

The eigen energy is given by

$$E_k = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m\rho^2}\left(n - \frac{\Phi_a}{2\Phi_0}\right)^2.$$

The energy eigenvalue for the ground states is a periodic function of $\frac{\Phi_a}{2\Phi_0}$ as shown in Fig.1

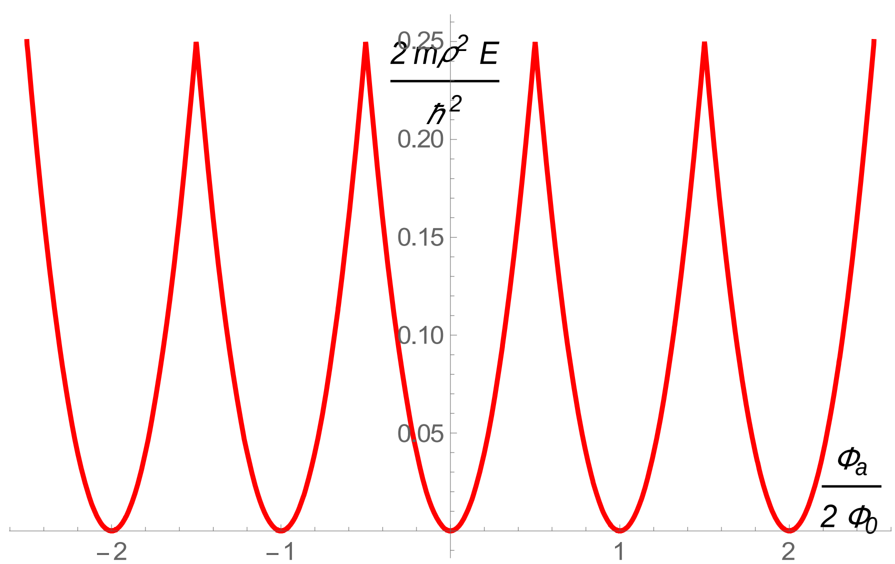


Fig.1 The ground state energy as s function of $\frac{\Phi_a}{2\Phi_0}$.

A.3 Approach from the Bloch theorem: Persistent current in conducting metallic ring

This was, in part, anticipated in a widely known but unpublished piece of work by Felix Bloch in the early thirties, who argued that the equilibrium free energy of a metallic circuit must be a periodic function of the flux through the circuit with period hc/e; this was jokingly known as a theorem which disproved all theories of the metastable current in superconductors. (from a book written by D.J. Thouless[12]).

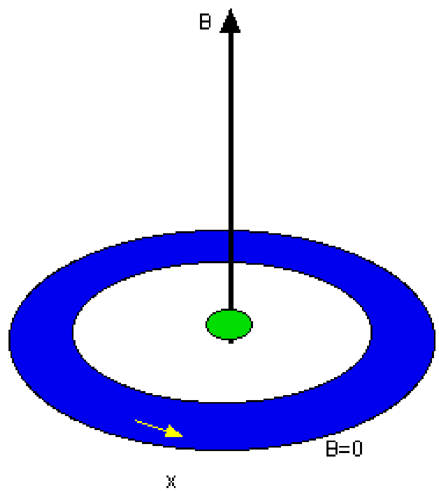


Fig. Circular conducting metal wire (one-dimensional along the *x* axis). The coordinate *x* is along the circular ring. The magnetic field is located only at the center (green part) of the ring (the same configuration as the Aharonov-Bohm effect). $L = 2\pi\rho$ (ρ: radius of the metal circular ring). Φ_a is the total magnetic flux penetrating the ring at the center.

(a) Bloch theorem and energy band

We consider a circular metal ring. A magnetic field is located only at the center of the ring (the same configuration as the Aharonov-Bohm effect). We assume that $q = -e$ ($e>0$). There is no magnetic field on the conducting metal ring ($\boldsymbol{B} = 0$). In other word, the magnetic flux exists only at the center. The vector potential $\boldsymbol{A}$ is related to $\boldsymbol{B}$ by

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} = 0,$$

or

$$\boldsymbol{A} = \nabla \chi .$$

The scalar potential χ is described by

$$\chi(x) = \int_{x_0}^{x} dx A(x),$$

where the direction of x is along the circular ring and x_0 is an arbitrary initial point in the ring. We now consider the gauge transformation. $\boldsymbol{A}$' and $\boldsymbol{A}$ are the new and old vector potentials, respectively. ψ' and ψ are the new and old wave functions, respectively.

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla(-\chi) = 0,$$

$$\psi'(\boldsymbol{r}) = \exp(\frac{ie\chi}{\hbar c})\psi(\boldsymbol{r}). \qquad \text{(Gauge transformation of the wave function)}$$

Since $\boldsymbol{A}$' = 0, ψ' is the field-free wave function and satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi' = i\hbar\frac{\partial}{\partial t}\psi'.$$

In summary, we have

$$\psi(x) = \psi'(x)\exp[-\frac{ie}{\hbar c}\int_{x_0}^{x} A(x)dx],$$

$$\psi(x+L) = \psi'(x+L)\exp[-\frac{ie}{\hbar c}\int_{x_0}^{x+L} A(x)dx],$$

where L is a perimeter of the circular metal wire ring. From these equation we get

$$\begin{aligned}\frac{\psi(x+L)}{\psi(x)} &= \frac{\psi'(x+L)}{\psi'(x)}\exp[-\frac{ie}{\hbar c}\int_{x}^{x+L} A(x)dx] \\ &= \frac{\psi'(x+L)}{\psi'(x)}\exp[-\frac{ie\Phi_a}{\hbar c}]\end{aligned}.$$

Here we use the relation

$$\int_{x}^{x+L} A(x)dx = \oint(\nabla\times A)\cdot d\boldsymbol{a} = \Phi_a,$$

where Φ_a is the total magnetic flux penetrating the ring at the center. It is reasonable to assume the periodic boundary condition

$$\psi'(x+L) = \psi'(x),$$

for the free particle wave function. Then we have

$$\psi(x+L) = \psi(x)\exp(-\frac{ie\Phi_a}{\hbar c}) = \exp(ikL)\psi(x) .$$

with the wavenumber

$$k = -\frac{e\Phi_a}{\hbar cL} = -\frac{2\pi}{L}\frac{\Phi_a}{2\Phi_0} .$$

This equation indicates that $\psi(x)$ is the Bloch wave function. The electronic energy spectrum of the system has a band structure. We now consider the case of k+G with

$$G = \frac{2\pi}{L} = \frac{2\pi}{2\pi\rho} = \frac{1}{\rho} ,$$

$$\exp[i(k+G)L]\psi(x) = \exp(ikL)\psi(x) = \psi(x+L) ,$$

since $\exp(iGL) = 1$. Therefore we have the periodicity of the energy eigenvalue

$$E(k+G) = E(k) , \qquad \text{or} \qquad E(\frac{\Phi_a}{2\Phi_0} + n) = E(\frac{\Phi_a}{2\Phi_0}) .$$

From the Bloch theory, we can also derive

$$E(-k) = E(k) , \qquad \text{or} \qquad E(-\frac{\Phi_a}{2\Phi_0}) = E(\frac{\Phi_a}{2\Phi_0}) .$$

The energy $E(k)$ depends on $\frac{\Phi_a}{2\Phi_0}$. It is actually a periodic function of $\frac{\Phi_a}{2\Phi_0}$ with the periodicity 1.

$$G = \frac{2\pi}{L} = 2\frac{e\Phi_0}{\hbar cL} ,$$

The magnetization $M(\Phi_a)$ is defined as

$$M(\Phi_a) = -\frac{\partial E(\Phi_a)}{\partial B} = -A\frac{\partial E(\Phi_a)}{\partial \Phi_a} = \frac{Ae}{\hbar cL}\frac{\partial E(k)}{\partial k} , \qquad (99)$$

where A (= $\pi\rho^2$) is the total area of the circular ring. This is proportional to the group velocity defined by

$$v_k = \frac{1}{\hbar}\frac{\partial E(k)}{\partial k}. \qquad (100)$$

The magnetic moment $M(\Phi_a)$ is related to the current flowing in the ring as

$$M(\Phi_a) = \frac{1}{c} I(\Phi_a) A = -A\frac{\partial E(\Phi_a)}{\partial \Phi_a}, \qquad (101)$$

or

$$I(\Phi_a) = -c\frac{\partial E(\Phi_a)}{\partial \Phi_a}. \qquad (102)$$

(b) Derivation of $E(\Phi_a)$

We consider the persistent current system in the ring in the presence of magnetic flux. $L = 2\pi\rho$.

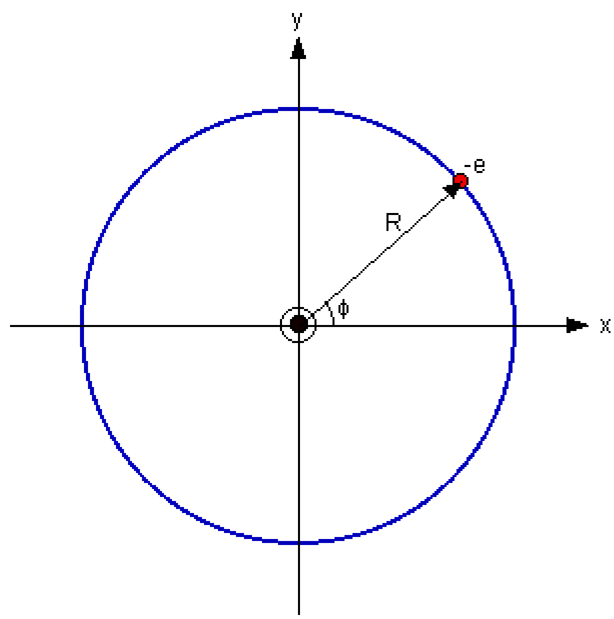


Fig. Circular conducting ring with radius $R = \rho$. The magnetic field ***B*** is located only at the center and is along the *z* axis (out of the page).

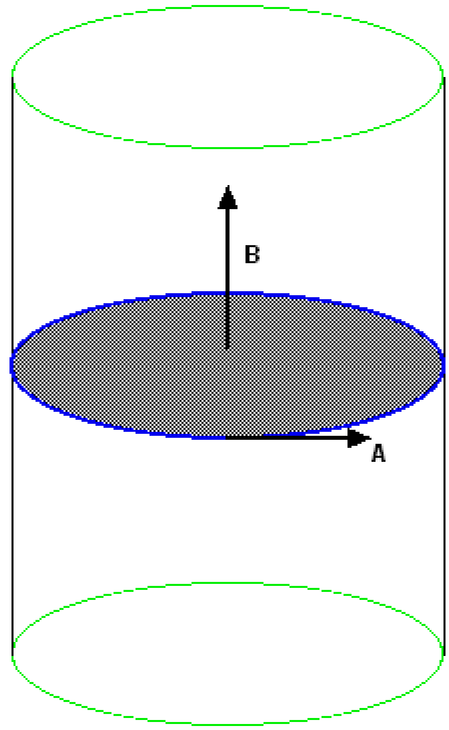


Fig. The vector potential $\boldsymbol{A}$ is along the $\boldsymbol{e}_\phi$ direction. The magnetic field is along the cylindrical axis (z axis) and is located only at the center of cylinder.

An electron is constrained to move on a 1D ring of radius ρ. At the center of the ring, there is a constant magnetic flux in the z direction. The magnetic flux through the surface bounded by the ring

$$\Phi_a = \oint (\nabla \times \boldsymbol{A}) \cdot d\boldsymbol{a} = \oint \boldsymbol{B} \cdot d\boldsymbol{a} .$$

Using Stoke's theorem,

$$\oint (\nabla \times \boldsymbol{A}) \cdot d\boldsymbol{a} = \oint \boldsymbol{A} \cdot d\ell = \oint \boldsymbol{B} \cdot d\boldsymbol{a} = \Phi_a .$$

From the azimuthal symmetry of the system, the magnitude of the azimuthal component of $\boldsymbol{A}$ must be the same everywhere along the path (radius ρ)

$$\boldsymbol{A} = \frac{\Phi_a}{2\pi\rho} \boldsymbol{e}_\phi . \tag{103}$$

Now we consider the Schrödinger equation for electron (q = -e) constrained to move on the ring, we have

$$\rho = \text{constant, and } z = \text{constant.}$$

We use the new vector potential

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi = 0,$$

or

$$A_\phi' = A_\phi + \frac{1}{\rho}\frac{\partial}{\partial\phi}\chi = 0,$$

or

$$0 = \frac{\Phi_a}{2\pi\rho} + \frac{1}{\rho}\frac{\partial\chi}{\partial\phi} = 0,$$

or

$$\chi = -\frac{\Phi_a}{2\pi}\phi .$$

The Hamiltonian is given by

$$\hat{H} = \frac{1}{2m}(\hat{\boldsymbol{p}} + \frac{e}{c}\boldsymbol{A}')^2 = \frac{1}{2m}\hat{\boldsymbol{p}}^2 .$$

The Schrödinger equation is given by

$$\langle \boldsymbol{r}|\hat{H}|\psi'\rangle = E\langle \boldsymbol{r}|\psi'\rangle,$$

or

$$\langle \boldsymbol{r}|\hat{H}|\psi\rangle = -\frac{\hbar^2}{2m}\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\psi'(\boldsymbol{r}) = E\psi'(\boldsymbol{r}),$$

or

$$\frac{\partial^2}{\partial\phi^2}\psi'(\boldsymbol{r}) = -\lambda^2\psi'(\boldsymbol{r}), \qquad (104)$$

where

$$\lambda = \sqrt{\frac{2mE}{\hbar^2}\rho^2} . \qquad (105)$$

Then the wave function is obtained as

$$\psi'(\phi) = \frac{1}{\sqrt{2\pi\rho}} e^{i\lambda\phi} . \tag{106}$$

The old wave function is related to the new wave function (q = -e, gauge transformation) by

$$\begin{aligned}
\psi(\phi) &= \exp(-\frac{iq\chi}{c\hbar})\psi'(\phi) \\
&= \exp(-\frac{ie\Phi_a\phi}{2\pi c\hbar})\frac{1}{\sqrt{2\pi\rho}}\exp(i\lambda\phi) \\
&= \frac{1}{\sqrt{2\pi\rho}}\exp[i(\lambda - \frac{e\Phi_a}{2\pi c\hbar})\phi] \\
&= \frac{1}{\sqrt{2\pi\rho}}\exp(i\mu\phi)
\end{aligned} . \tag{107}$$

where

$$\mu = \lambda - \frac{e\Phi_a}{2\pi c\hbar}$$

From the periodic boundary

$$\psi(\phi + 2\pi) = \psi(\phi) , \tag{108}$$

we have

$$2\pi\mu = 2\pi(\lambda - \frac{e\Phi_a}{2\pi c\hbar}) = -2n\pi \text{ (}n\text{: integer),}$$

or

$$\mu = \lambda - \frac{e\Phi_a}{2\pi c\hbar} = -n . \tag{109}$$

Here we define the quantum fluxoid Φ_0 as

$$\Phi_0 = \frac{\pi c\hbar}{e} = 2.06783372 \text{ x } 10^{-7} \text{ Gauss cm}^2 \text{ (from the NIST Website)}$$

then we have

$$\lambda = \sqrt{\frac{2mE}{\hbar^2}\rho^2} = \frac{\Phi_a}{2\Phi_0} - n .$$

Then the energy eigenvalue is obtained as

$$E = \frac{\hbar^2}{2m\rho^2}\left(\frac{\Phi_a}{2\Phi_0} - n\right)^2.$$

The energy eigenvalue of the ground states is shown in **Fig.1**.

We now consider the current density ***J*** defined by (quantum mechanics)

$$\boldsymbol{J} = \frac{q\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{q^2}{mc}\boldsymbol{A}\psi^*\psi],$$

where

$$\boldsymbol{A} = \frac{\Phi_a}{2\pi\rho}\boldsymbol{e}_\phi,$$

$$\psi(\phi) = \frac{1}{\sqrt{2\pi\rho}}e^{i\mu\phi},$$

$$\nabla\psi(\phi) = \boldsymbol{e}_\phi\frac{1}{\rho}\frac{\partial}{\partial\phi}\psi(\phi),$$

with

$\mu = \lambda - \dfrac{e\Phi_a}{2\pi c\hbar}$, and $q = -e$ (electron)

Then we have

$$\begin{aligned}\boldsymbol{J} &= -e\left(\frac{\hbar\mu}{2\pi m\rho^2} + \frac{e\Phi_a}{4\pi^2 mc\rho^2}\right)\boldsymbol{e}_\phi \\ &= -e\left[\frac{\hbar}{2\pi m\rho^2}\left(\lambda - \frac{e\Phi_a}{2\pi c\hbar}\right) + \frac{e\Phi_a}{4\pi^2 mc\rho^2}\right]\boldsymbol{e}_\phi, \\ &= -\frac{e\hbar\lambda}{2\pi m\rho^2}\boldsymbol{e}_\phi\end{aligned}$$

or

$$J_\phi = \frac{e\hbar}{2\pi m\rho^2}\left(-\frac{\Phi_a}{2\Phi_0} + n\right).$$

This is compared with

$$\frac{\partial E}{\partial \Phi} = \frac{\hbar^2}{m\rho^2}\frac{1}{2\Phi_0}(\frac{\Phi_a}{2\Phi_0} - n) = \frac{e\hbar}{2\pi mc\rho^2}(\frac{\Phi_a}{2\Phi_0} - n),$$

or

$$J_\phi = -c\frac{\partial E}{\partial \Phi} = \frac{e\hbar}{2\pi m\rho^2}(-\frac{\Phi_a}{2\Phi_0} + n).$$

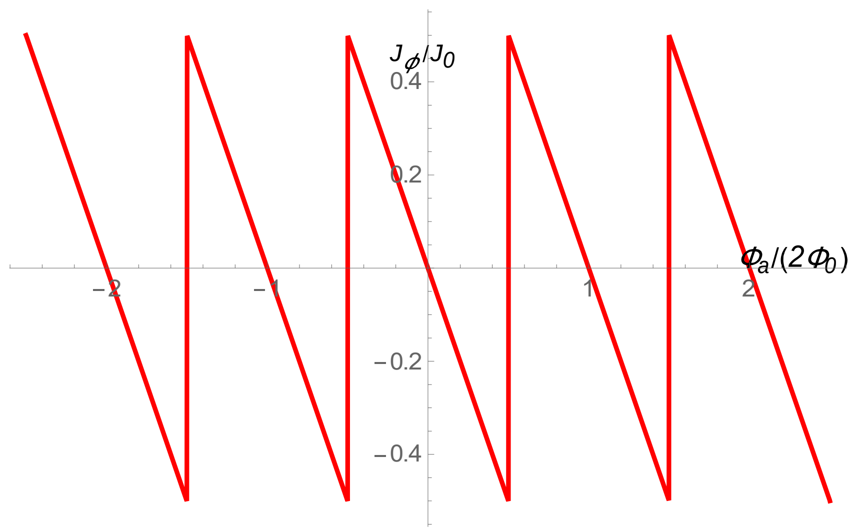


Fig. The persistent current density J_ϕ / J_0 as a function of $\frac{\Phi_a}{2\Phi_0}$. $J_0 = e\hbar / 2\pi m\rho^2$.

APPENDIX III

S. Washburn, Aharonov-Bohm effects in loops of gold
Chapter 1 p.3-36
B.L. Altshuler, P.A. Lee, and R,A, Webb, Mesoscopic Phenomena in Solids (North-Holland, 1991)

The Aharonov-Bohm effect has been confirmed in the conduction phenomena in mesoscopic system such as a ring made of gold wire. Washburn et al. (IBM) prepared a metal ring with a diameter 1 μm, which is made of gold thin wires. An external magnetic field is applied along a direction perpendicular to the loop surface. They measure the magnetoresistance of the loop of gold. The result of the conductance (reciprocal of the magnetoresistance) is shown as a function of the magnetic field (B). The data seems a random signal. This signal arises from the interference of electrons flowing on the right hand of the loop and the left hand of the loop. This interference is related to the magnetic flux passing through the loop. Over the modest ranges of field, the resistance oscillates with the flux period $2\Phi_0$. The conductance G can be expressed by

$$G = G_0 + \sum_n G_n \cos(2\pi n \frac{BA}{2\Phi_0})$$

The angular frequency of the first harmonics;

$$\omega_1 = \frac{A}{2\Phi_0} = \frac{\pi r_0^{\ 2}}{\frac{\hbar c}{e}} = 8.12144 \text{ x } 10^{-2}$$

Then we have the frequency

$$f_1 = \frac{\omega_1}{2\pi} = \frac{\pi r_0^{\ 2}}{2\pi \frac{\hbar c}{e}} = 129.257 \text{ (1/T)}$$

where A is the area enclosed. The sample diamter is 825 nm. The oscillation can be analyzed by the Fourier transform. The peak appears at 129.257 (1/T). Since the current has a sawtooth shape as a function of B (or Φ_a), the Fourier spectrum has higher harmonoics at $2f_1$, $3f_1$, and so on, depending on the nonlinearity of the current shape. Note that the peak at $2f_1$ does not show the evidence of the quantum fluxoide (Φ_0).

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