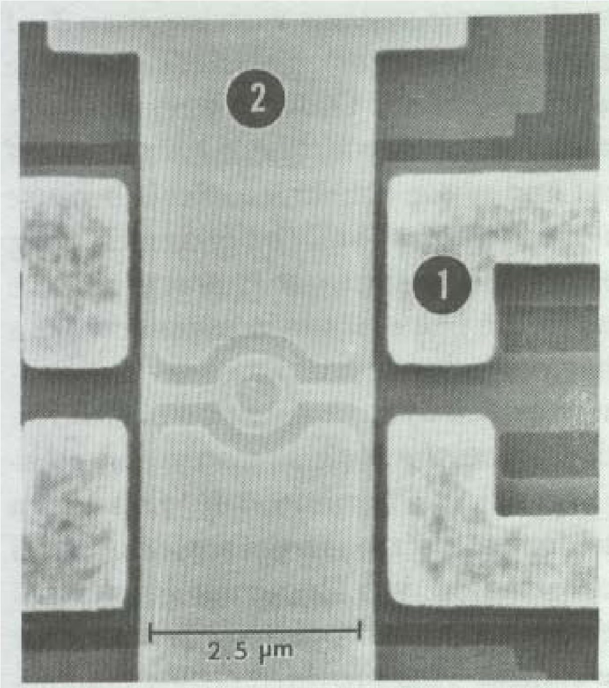
Advanced Quantum Physics

Lecture 9



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Section 3:Relativity and Magnetic fields

Hamiltonian in an electromagnetic field (1)

- See how electromagnetic fields are introduced into Classical mechanics using Hamiltonian formulation.
- Two of the Maxwell equations: $\nabla \cdot \mathbf{B} = 0 \qquad \nabla \times \boldsymbol{\varepsilon} = -\frac{\partial \mathbf{B}}{\partial t}$

- Since $\nabla \cdot \nabla \times \mathbf{a} = 0$ for any $\mathbf{a}$ and $\nabla \cdot \mathbf{B} = 0$ define $\mathbf{B}$ in terms of vector potential $\mathbf{A}$ by: $\mathbf{B} = \nabla \times \mathbf{A}$

- Using Faraday's law: $\nabla \times \boldsymbol{\varepsilon} = -\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \frac{\partial \mathbf{A}}{\partial t} \Rightarrow \nabla \times \left(\boldsymbol{\varepsilon} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0$

- Given $\nabla \times \nabla \phi = 0$ where ϕ is a scalar potential $\Longrightarrow \boldsymbol{\varepsilon} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \phi$
- Thus we can express $\boldsymbol{\varepsilon}$ & $\mathbf{B}$ in terms of $\mathbf{A}$ and ϕ by:

$$\mathbf{B} = \nabla \times \mathbf{A}, \qquad \boldsymbol{\varepsilon} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t}.$$

Hamiltonian in an electromagnetic field (2)

- Choice of $\mathbf{A}$ and ϕ not unique, we can transform them:

$$\begin{cases} \mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla f(\mathbf{r}, t) \\ \phi \to \phi' = \phi - \dfrac{\partial f}{\partial t} \end{cases}$$

- Does not affect the fields and forces, called *gauge invariance* - can often be used to simplify problems.

- Hamiltonian in Schrodinger eqn. based on classical dynamics:

- Classical Hamiltonian - kinetic and potential energies, $H = T + V$

system of N particles, coordinates x_j momenta p_j $\quad j = 1, 2, 3 \cdots N$

H function of x_j, p_j eqs. of motion: $\dfrac{dx_j}{dt} = \dfrac{\partial H}{\partial p_j} \;\; ; \;\; \dfrac{dp_j}{dt} = -\dfrac{\partial H}{\partial x_j}$

- Check results: for single particle moving in potential $V(x_j)$

$$H = \frac{\sum p_j^2}{2m} + V(x_j) \Rightarrow \underbrace{\frac{dx_j}{dt} = \frac{p_j}{m}}_{p = mv} \;\; ; \;\; \underbrace{\frac{dp_j}{dt} = -\frac{\partial V}{\partial x_j}}_{F = ma}.$$

Equivalent to: $p = mv$ $\quad F = ma$

Hamiltonian in an electromagnetic field (3)

- Classically to introduce EM field we replace p_j by $(p_j - qA_j)$ in H this gives the expected result since:

$$H = \frac{\sum (p_j - qA_j)^2}{2m} + q\phi = \frac{p^2}{2m} - \frac{q}{m}\mathbf{p}\cdot\mathbf{A} + \frac{q^2}{2m}A^2 + q\phi\,,$$

the equation of motion are:

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j} = \frac{p_j}{m} - \frac{qA_j}{m}$$

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j} = \frac{q}{m}\mathbf{p}\cdot\frac{\partial \mathbf{A}}{\partial x_j} - \frac{q^2}{m}\mathbf{A}\cdot\frac{\partial \mathbf{A}}{\partial x_j} - q\frac{\partial \phi}{\partial x_j}$$

$$= \frac{q}{m}(\mathbf{p} - q\mathbf{A})\cdot\frac{\partial \mathbf{A}}{\partial x_j} - q\frac{\partial \phi}{\partial x_j}$$

$$m\frac{d^2 x_j}{dt^2} = \frac{dp_j}{dt} - q\frac{dA_j}{dt}$$

$$= \frac{dp_j}{dt} - q\left[\frac{\partial A_j}{\partial t} + \sum_k \frac{\partial A_j}{\partial x_k}\frac{dx_k}{dt}\right]$$

Hamiltonian in an electromagnetic field (4)

- Previous slide:

$$m\frac{d^2x_j}{dt^2}=\frac{dp_j}{dt}-q\left[\frac{\partial A_j}{\partial t}+\sum_k\frac{\partial A_j}{\partial x_k}\frac{dx_k}{dt}\right]$$

$$\frac{dp_j}{dt}=\frac{q}{m}(\mathbf{p}-q\mathbf{A})\cdot\frac{\partial \mathbf{A}}{\partial x_j}-q\frac{\partial\phi}{\partial x_j}$$

$$m\frac{d^2x_j}{dt^2}=q\underbrace{\left(\frac{\mathbf{p}-q\mathbf{A}}{m}\right)}_{\mathbf{v}}\cdot\frac{\partial \mathbf{A}}{\partial x_j}-q\frac{\partial\phi}{\partial x_j}-q\left[\frac{\partial A_j}{\partial t}+\sum_k\frac{\partial A_j}{\partial x_k}\frac{dx_k}{dt}\right]$$

$$m\frac{d^2x_j}{dt^2}=-q\underbrace{\left(\frac{\partial\phi}{\partial x_j}+\frac{\partial A_j}{\partial t}\right)}_{=-\mathcal{E}_j}+q\underbrace{\sum_k v_k\left[\frac{\partial A_k}{\partial x_j}-\frac{\partial A_j}{\partial x_k}\right]}_{=(\mathbf{v}\times\nabla\times\mathbf{A})_j=(\mathbf{v}\times\mathbf{B})_j}$$

$$\mathbf{B}=\nabla\times\mathbf{A},\boldsymbol{\varepsilon}=-\nabla\phi-\frac{\partial\mathbf{A}}{\partial t}\Rightarrow$$

- Hence we obtain the equation of motion for a particle in fields $\boldsymbol{\varepsilon},\mathbf{B}$

$$m\ddot{\mathbf{r}}=q\boldsymbol{\varepsilon}+q\,\mathbf{v}\times\mathbf{B}$$

Quantum Mechanics in an electromagnetic field (1)

- Following the same procedure in QM, replacing $\hat{\mathbf{p}}$ by $\hat{\mathbf{p}} - q\mathbf{A}$

$$\hat{H}\psi = \tfrac{1}{2m}\left(\hat{\mathbf{p}} - q\mathbf{A}\right)^2\psi + q\phi\psi = i\hbar\frac{\partial\psi}{\partial t}$$

and with $\hat{\mathbf{p}} = -i\hbar\nabla$ Schrodinger's equation becomes:

$$\hat{H}\psi = \frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}\right)^2\psi + q\phi\psi = i\hbar\frac{\partial\psi}{\partial t}$$

- We showed earlier that a change of gauge does not affect the $\boldsymbol{\varepsilon}, \mathbf{B}$ fields
- But is the Schrodinger equation invariant?
- Apply a gauge transformation to the potentials: -

$$\begin{cases} \mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla f(\mathbf{r}, t) \\ \phi \rightarrow \phi' = \phi - \dfrac{\partial f}{\partial t} \end{cases}$$

- The Schrodinger equation becomes:

$$\hat{H}\psi = \frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}' + q\nabla f\right)^2\psi + q\phi'\psi + q\frac{\partial f}{\partial t}\psi = i\hbar\frac{\partial\psi}{\partial t}$$

- Define a new wavefunction: $\psi' = \psi e^{i\Lambda(\mathbf{r},t)}$ with a phase factor $\Lambda(\mathbf{r}, t)$
- Note that $\psi'^*\psi' = \psi\psi^*$ so the probability density is invariant.

Quantum Mechanics in an electromagnetic field (2)

- From the last slide: $\psi' = \psi e^{i\Lambda(\mathbf{r},t)} \Rightarrow \psi = \psi' e^{-i\Lambda(\mathbf{r},t)}$ substituting into the Schrodinger equation:

$$\underbrace{\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}' + q\nabla f\right)^2 \psi' e^{-i\Lambda}}_{} + q\phi'\psi' e^{-i\Lambda} + q\frac{\partial f}{\partial t}\psi' e^{-i\Lambda} = i\hbar\frac{\partial(\psi' e^{-i\Lambda})}{\partial t}$$

Given: $\psi = \psi' e^{-i\Lambda(\mathbf{r},t)} \Rightarrow$

$$-i\hbar\nabla(e^{-i\Lambda}\psi') = -\hbar e^{-i\Lambda}(\nabla\Lambda)\psi' - i\hbar e^{-i\Lambda}\nabla\psi'$$

Kinetic energy term

$$\overbrace{\frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}' + q\nabla f\right)\left(-i\hbar\nabla - q\mathbf{A}' + q\nabla f\right)\psi' e^{-i\Lambda}}^{}$$

$$= \frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}' + q\nabla f\right)e^{-i\Lambda}\left(-\hbar(\nabla\Lambda)\psi' - i\hbar\nabla\psi' - q\mathbf{A}'\psi' + q\nabla f\psi'\right)$$

$$= \frac{1}{2m}e^{-i\Lambda}\left(-\hbar(\nabla\Lambda) - i\hbar\nabla - q\mathbf{A}' + q\nabla f\right)^2\psi'$$

Quantum Mechanics in an electromagnetic field (3)

- From the last slide Schrodinger eqn:

$$\frac{1}{2m}e^{-i\Lambda}\left(-\hbar(\nabla\Lambda)-i\hbar\nabla-q\mathbf{A}'+q\nabla f\right)^2\psi'+q\phi'\psi'e^{-i\Lambda}+q\frac{\partial f}{\partial t}\psi'e^{-i\Lambda}=i\hbar\frac{\partial(\psi'e^{-i\Lambda})}{\partial t}$$

- Given $\psi=\psi' e^{-i\Lambda(\mathbf{r},t)} \Rightarrow \frac{\partial\psi}{\partial t}=\frac{\partial}{\partial t}\left(e^{-i\Lambda}\psi'\right)=-i\frac{\partial\Lambda}{\partial t}e^{-i\Lambda}\psi'+e^{-i\Lambda}\frac{\partial\psi'}{\partial t}$

- Substituting into the Schrodinger eqn. above:

$$\frac{1}{2m}e^{-i\Lambda}\left(\underbrace{-\hbar(\nabla\Lambda)}_{1}-i\hbar\nabla-q\mathbf{A}'\underbrace{+q\nabla f}_{2}\right)^2\psi'+q\phi'\psi'e^{-i\Lambda}\underbrace{+q\frac{\partial f}{\partial t}\psi'e^{-i\Lambda}}_{3}$$

$$=\underbrace{\hbar\frac{\partial\Lambda}{\partial t}\psi'e^{-i\Lambda}}_{4}+i\hbar\frac{\partial\psi'}{\partial t}e^{-i\Lambda}$$

If $\Lambda=\frac{q}{\hbar}f$ 1 & 2 cancel, 3 & 4 cancel

$e^{-i\Lambda}$ cancels

$$\Rightarrow \hat{H}\psi'=\frac{1}{2m}\left(-i\hbar\nabla-q\mathbf{A}'\right)^2\psi'+q\phi'\psi'=i\hbar\frac{\partial\psi'}{\partial t}$$

Original Sch. Eqn.
With $\mathbf{A}',\phi',\psi'$
replacing $\mathbf{A},\phi,\psi$

Quantum Mechanics in an electromagnetic field (4)

- From the last slide:

$$\hat{H}\psi' = \frac{1}{2m}\left(-i\hbar\nabla - q\mathbf{A}'\right)^2 \psi' + q\phi'\psi' = i\hbar\frac{\partial\psi'}{\partial t}$$

- Schrodinger eqn. is gauge invariant under the following transformation;

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla f(\mathbf{r}, t), \qquad \phi \to \phi' = \phi - \frac{\partial f}{\partial t}, \quad \psi' = \psi e^{i\Lambda(\mathbf{r},t)}$$

given that we introduce a phase factor $\Lambda = \frac{q}{\hbar} f$ into the wavefunction.

- Expanding the Hamiltonian in the Schrodinger equation:

$$\hat{H}\psi = \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})(-i\hbar\nabla\psi - q\mathbf{A}\psi) + q\phi\psi$$

- And using:

$$\nabla\cdot\left(\mathbf{A}\psi\right) = \mathbf{A}\cdot\left(\nabla\psi\right) + \left(\nabla\cdot\mathbf{A}\right)\psi$$

- We get:

$$\hat{H}\psi = \frac{1}{2m}\left[-\hbar^2\nabla^2\psi + i\hbar q(2\mathbf{A}\cdot\nabla\psi + \psi\nabla\cdot\mathbf{A}) + q^2A^2\psi\right] + q\phi\psi.$$

- For the gauges used most often (*Coulomb* and *Landau*) $\nabla\cdot\mathbf{A} = 0$.
If the fields are weak it is sometimes possible to neglect the term in A^2.

The Aharonov-Bohm effect* (1)

- In classical physics only $\boldsymbol{\varepsilon}$ and $\mathbf{B}$ are physically significant, the potentials $\mathbf{A}$ and ϕ can be altered by a gauge transformation.
- Quantum mechanics is different….. with a gauge transformation:

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla f(\mathbf{r}, t), \qquad \phi \to \phi' = \phi - \frac{\partial f}{\partial t}$$

- A wavefunction transforms $\psi \to \psi' = \psi e^{i\Lambda(\mathbf{r},t)}$ where $\Lambda(\mathbf{r},t) = \frac{q}{\hbar} f(\mathbf{r},t)$
- If $\mathbf{A}(\mathbf{r}) = \nabla f(\mathbf{r}) = \frac{\hbar}{q} \nabla \Lambda(\mathbf{r})$ then $\mathbf{B} = \nabla \times \mathbf{A} = 0$

and $\Lambda(\mathbf{r}) = \frac{q}{\hbar} \int_a^b \mathbf{A}(\mathbf{r}') \cdot d\,\mathbf{r}'$ - a line integral between points a and b.

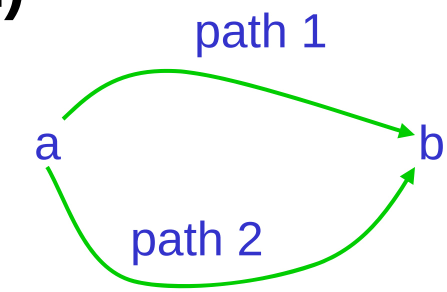
- Hence

$$\psi(\mathbf{r}) = \psi(\mathbf{r}_0) \exp\left(i \frac{q}{\hbar} \int_a^b \mathbf{A}(\mathbf{r}') \cdot d\,\mathbf{r}' \right)$$

- This suggest that when a charged particle moves through a region where $\mathbf{B} = 0$ but $\mathbf{A} \neq 0$ it undergoes a quantum mechanical phase change.

*Aharonov & Bohm Phys Rev **115**,485 (1959)

The Aharonov-Bohm effect (2)



- Charged particle moves around a closed loop along path 1 from point a to point b, returning along path 2 from point b to point a.

- Phase change: $\frac{q}{\hbar}\int_{path1} \mathbf{A}\cdot d\,\mathbf{r}' - \frac{q}{\hbar}\int_{path2} \mathbf{A}\cdot d\,\mathbf{r}' = \frac{q}{\hbar}\oint_{loop} \mathbf{A}\cdot d\,\mathbf{r}'$

- By Stoke's theorm: $\oint_{loop} \mathbf{A}\cdot d\,\mathbf{r}' = \iint_{\substack{enclosed\\surface}} \nabla\times\mathbf{A}\cdot d\mathbf{S} = \iint_{\substack{enclosed\\surface}} \mathbf{B}\cdot d\mathbf{S} = \Phi$

- Φ is the magnetic flux threading the closed loop.

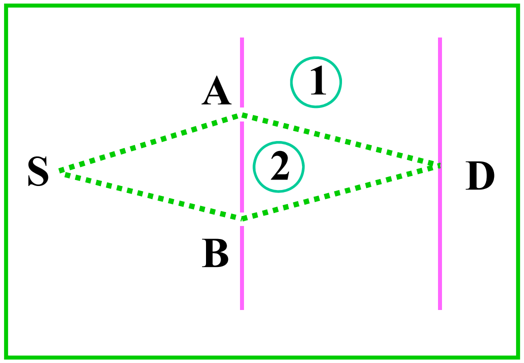
- Wavefunction phase change as particle traverses loop: $\delta\Lambda = \frac{q}{\hbar}\Phi.$

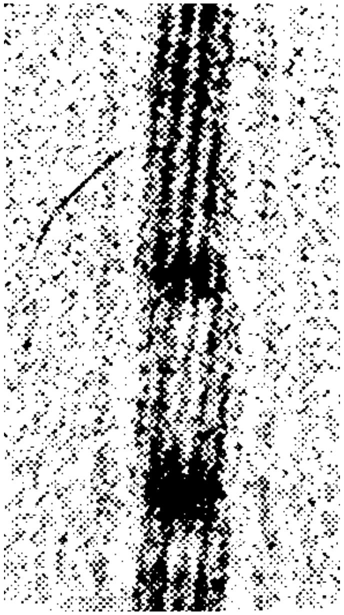
- For loops not enclosing magnetic flux – no phase change.

- However if a charged particle moves in a region where $\mathbf{A}\neq 0$ it's phase will change – even if $\mathbf{B}=0$ throughout the path.

The Aharonov-Bohm effect (3)

- •Illustrated by a diffraction experiment.
- •Charged particles from S impinge on a screen with two slits A,B. An inteference pattern is detected at D.
- •If a solenoid carrying flux (none of which escapes..) is placed in position 1 there is no change to the pattern.
- •If placed in position 2 the pattern changes – how much depends on the flux.
- •Image on the right - first observation of this effect.
- •A magnetised whisker of iron was placed in position 2. The whisker tapered along it's length – varying the B field and magnetic flux.
- •The fringe pattern changes for different parts of the whisker – due to the different fluxes.
- •Possibility of 'escaping' flux - more conclusive expt. Tonomura et al Phys Rev Lett **56**,792 (1986).

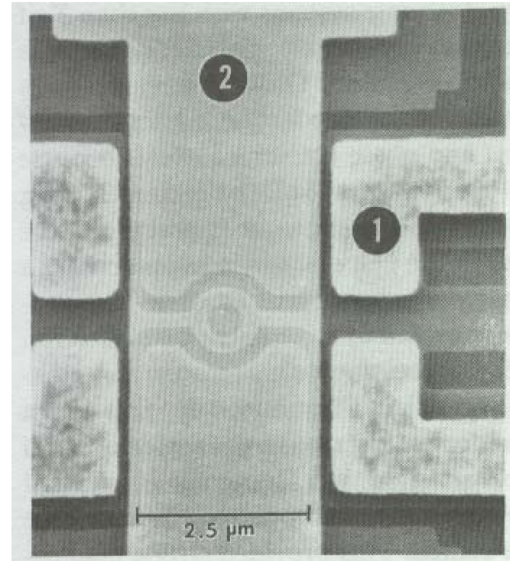


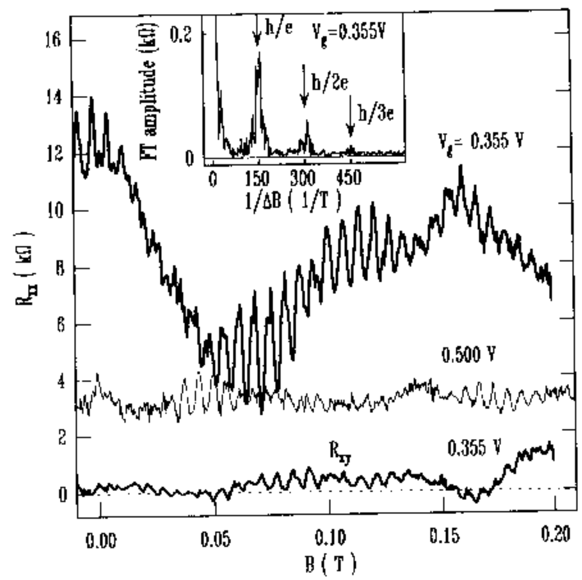


R G Chambers Phys Rev Lett **5**,3 (1960)

The Aharonov-Bohm effect (4)

- Effect observed in micron-scale metal and GaAs/AlGaAs semiconductor ring structures.
- Measurements made at low temperatures to reduce inelastic scattering from phonons.
- Observation of oscillations in resistance as a function of magnetic field - the varying flux threading the loop causes phase changes.
- Between peaks, change in magnetic flux causes electron phase to vary by 2π.
- $\delta\Lambda = \frac{q}{\hbar}\Phi = \frac{q}{\hbar}BA$ -from this we can calculate size of loop – see example!
- On Fourier transforming results, ‘harmonics’ appear at 2x and 3x fundamental.
- Harmonics due to electrons travelling 2x and 3x around ring to pick up a phase change of 2π & interfere constructively.





Lee et al Appl Phys Lett **55**,625 (1989)

Quantization of magnetic flux

•Hollow cylinder made of superconductor in ‘normal’ state and a magnetic field.

•Cool cylinder below critical temperature - becomes superconducting - expels field (‘Meissner effect’ - B=0 inside material).

•Reduce external field to zero.

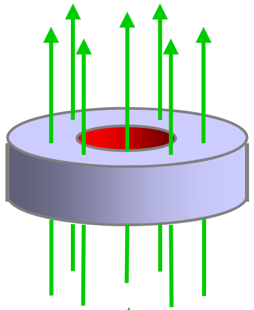
•Magnetic flux trapped in centre of cylinder.

•Wavefunction single valued - around the ring- $\delta\Lambda = \frac{q}{\hbar}\Phi = 2n\pi$ -macroscopic quantum object!!

So flux inside ring is quantised with: $\Phi = \frac{2\pi\hbar}{q} n$

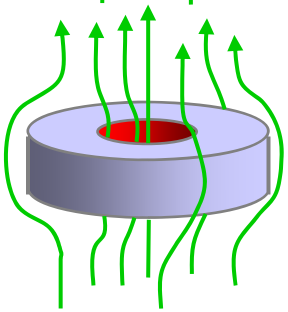
$T > T_c$

$B = B_1$



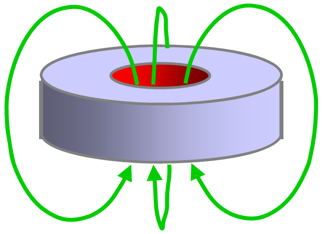
$T < T_c$

$B = B_1$



$T < T_c$

$B = 0$

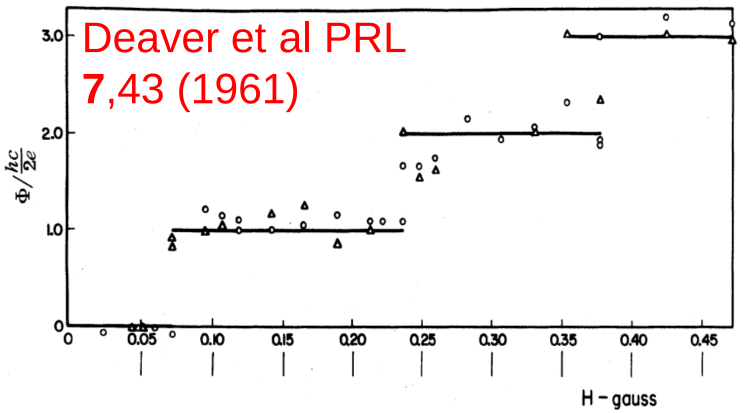


Experiment

•Superconducting hollow Sn cylinder cooled in different magnetic fields.

•Magnetic moment measured with vibrating magnetometer.

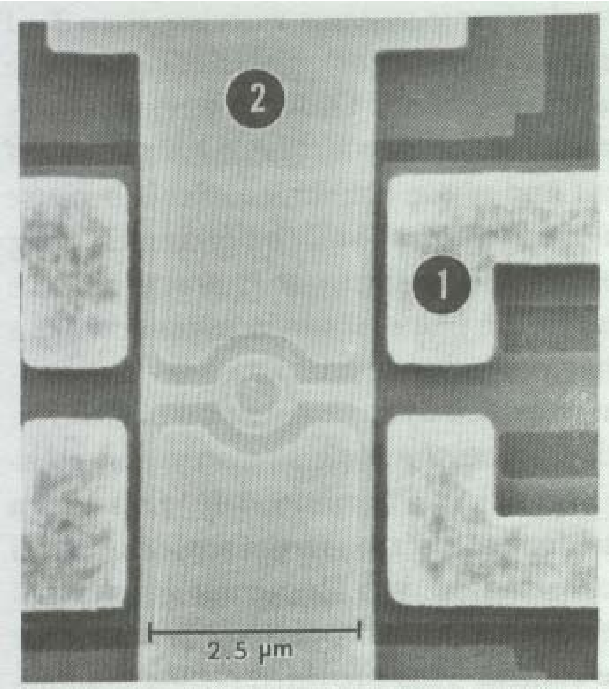
•Values quantised in units of $\frac{2\pi\hbar}{2e}$ - evidence for ‘Cooper pairs’



Lecture 9 - Summary

- Introducing electromagnetic fields into a classical Hamiltonian – the concept of *gauge invariance.*
- Adaptation of the Schrodinger equation to include electromagnetic fields (replace $\hat{\mathbf{p}}$ by $\hat{\mathbf{p}} - q\mathbf{A}$).
- Proof that Schrodinger equation is invariant under a gauge transformation provided we introduce a phase shift into the wavefunction.
- The Aharonov-Bohm effect – a charged particle moving in a path enclosing magnetic flux undergoes a change in it's quantum mechanical phase. Experimental evidence (i) electron diffraction around a magnetised metal whisker (ii) measurements of the resistance of a ring of semiconductor material.
- Measurement of the quantization of magnetic flux using a superconducting cylinder $\Phi = \frac{2\pi\hbar}{q} n$.

Lecture 9



The End!!

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