UNIVERSITY OF CAMBRIDGE

NST Part II Physics
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ADVANCED QUANTUM PHYSICS

Handout 3

- Gauge invariance (Aharanov-Bohm)
- Magnetic moments
- Stern-Gerlach
- Landau levels (Quantum Hall effect)

Charged particles in EM Fields

-- To obtain a quantum treatment of particle interactions with given electric and magnetic fields $\mathbf{E}(\mathbf{r},t)$, $\mathbf{B}(\mathbf{r},t)$, we shall :

- Assume that the *quantum* Hamiltonian describing such interactions has the same form as the non-relativistic *classical* Hamiltonian

- Add spin (magnetic moment) interactions with the $\mathbf{B}$ field "by hand"

  [spin and its interactions are predicted by the relativistically covariant Dirac equation, as will be discussed briefly later]

-- There are many implications and applications :

- In this handout: the Aharanov-Bohm effect, spin precession, the Stern-Gerlach experiment, Landau levels, ...

- Later: atomic structure, the Zeeman effect, the Stark effect, ...

Electrodynamics : classical → quantum

-- In classical electrodynamics, the motion of a charged particle is governed by the Lorentz force equation

$$m\ddot{\mathbf{r}} = q\mathbf{E} + q\mathbf{v} \wedge \mathbf{B} \tag{3.3.1}$$

-- The fields $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ can be expressed in terms of scalar and vector potentials $\phi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$ as

$$\mathbf{B} = \boldsymbol{\nabla} \wedge \mathbf{A} \; ; \qquad \mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \mathbf{A}}{\partial t}$$

-- In the Part II course "Electrodynamics and Optics", it is shown that equation (3.3.1) can be obtained from the classical Hamiltonian

$$\boxed{H = \frac{1}{2m}\left[\mathbf{p} - q\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t)} \tag{3.3.2}$$

The proof that equation (3.3.2) leads, via Hamilton's equations, to equation (3.3.1) is included for completeness as Appendix A

Electrodynamics : classical → quantum (2)

-- For a free particle (no EM field), the Hamiltonian is simply $H = \mathbf{p}^2/2m$

Comparing with equation (3.3.2), we see that interactions with an external EM field can be introduced via the "*minimal substitution*" prescription :

$$\boxed{\mathbf{p} \to \mathbf{p} - q\mathbf{A}\ ; \qquad E \to E + q\phi}$$

-- Assuming that the *quantum* Hamiltonian takes the same form as the classical Hamiltonian suggests adopting the operator

$$\boxed{\hat{H} = \frac{1}{2m}\left[\hat{\boldsymbol{p}} - q\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t)} \qquad (\hat{\boldsymbol{p}} = -i\hbar\boldsymbol{\nabla})$$

-- The time-dependent Schrödinger equation for a charged particle in a given electromagnetic field described by potentials $\mathbf{A}$ and ϕ is then

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}(\mathbf{r},t)\right]^2\psi + q\phi(\mathbf{r},t)\psi} \qquad \textbf{(3.4.1)}$$

Gauge Invariance

-- The choice of $\mathbf{A}$ and ϕ is not unique; a *gauge transformation*

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla} f \ ; \qquad \phi \to \phi' = \phi - \frac{\partial f}{\partial t}$$

where $f(\mathbf{r},t)$ is an arbitrary function, leaves $\mathbf{E}$ and $\mathbf{B}$ unchanged

$\rightarrow$ Maxwell's equations are *gauge invariant*

-- Is Schrödinger's equation gauge invariant also ?

Expressed in terms of the gauge-transformed (primed) potentials $\mathbf{A}'$ and ϕ', Schrödinger's equation (3.4.1) is

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla} f)\right]^2\psi + q\phi'\psi + q\frac{\partial f}{\partial t}\psi \qquad \textbf{(3.5.1)}$$

This does *not* have the same form as the original Schrödinger equation (the extra terms involving $f(\mathbf{r},t)$ do not cancel)

$\Rightarrow$ The answer would seem to be "*no*" (not gauge invariant)

Gauge Invariance (2)

-- The only hope of restoring gauge invariance is to transform the *wave-function* ψ as well as the potentials $\mathbf{A}$, ϕ :

$$\mathbf{A} \to \mathbf{A}' \; ; \quad \phi \to \phi' \; ; \quad \psi \to \psi'$$

To leave the probability density unchanged, $|\psi'|^2 = |\psi|^2$, the only realistic choice is to multiply the wavefunction ψ by a phase factor :

$$\boxed{\psi(\mathbf{r},t) \to \psi'(\mathbf{r},t) = \psi(\mathbf{r},t)e^{i\Lambda(\mathbf{r},t)}}$$

where $\Lambda(\mathbf{r},t)$ is an arbitrary function of position and time

-- Setting $\psi = \psi' e^{-i\Lambda(\mathbf{r},t)}$ in equation (3.5.1), the gauge-transformed (primed) version of Schrödinger's equation then becomes

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

(3.6.1)

Gauge Invariance (3)

-- In full, the first term on the right-hand side of equation (3.6.1) is

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

(3.7.1)

-- The identity

$$\begin{aligned}-i\hbar\boldsymbol{\nabla}(e^{-i\Lambda}\psi') &= -\hbar e^{-i\Lambda}(\boldsymbol{\nabla}\Lambda)\psi' - i\hbar e^{-i\Lambda}\boldsymbol{\nabla}\psi' \\ &= e^{-i\Lambda}\big(-\hbar(\boldsymbol{\nabla}\Lambda) - i\hbar\boldsymbol{\nabla}\big)\psi'\end{aligned}$$

allows the two rightmost factors in equation (3.7.1) to be written as

$$\begin{aligned}&\big(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla} f)\big)(e^{-i\Lambda}\psi') \\ &\qquad = e^{-i\Lambda}\big[-\hbar(\boldsymbol{\nabla}\Lambda) - i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla} f)\big]\psi'\end{aligned}$$

-- The equation above holds for *any* ψ', so we obtain the *operator* relation

$$\big(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla} f)\big)e^{-i\Lambda} = e^{-i\Lambda}\big[-\hbar(\boldsymbol{\nabla}\Lambda) - i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla} f)\big]$$

(3.7.2)

Gauge Invariance (4)

-- Equation (3.7.2) can be written schematically as

$$(\ldots)e^{-i\Lambda} = e^{-i\Lambda}[\ldots]$$

Pre-operating on both sides of the above equation by (…) then gives

$$\begin{aligned}(\ldots)^2 e^{-i\Lambda} &= (\ldots)e^{-i\Lambda}[\ldots] \\ &= e^{-i\Lambda}[\ldots][\ldots] = e^{-i\Lambda}[\ldots]^2\end{aligned}$$

Written out in full, this is

$$\big(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}f)\big)^2 e^{-i\Lambda} = e^{-i\Lambda}\big[-\hbar(\boldsymbol{\nabla}\Lambda) - i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}f)\big]^2$$

-- Hence equation (3.6.1) becomes

$$\begin{aligned}&e^{-i\Lambda}\hbar\frac{\partial\Lambda}{\partial t}\psi' + i\hbar e^{-i\Lambda}\frac{\partial\psi'}{\partial t} \\ &\qquad = e^{-i\Lambda}\left[\frac{1}{2m}\big[-\hbar(\boldsymbol{\nabla}\Lambda) - i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}f)\big]^2 + q\phi' + q\frac{\partial f}{\partial t}\right]\psi'\end{aligned}$$

Gauge Invariance (5)

-- Cancelling the overall pre-factors of $e^{-i\Lambda}$ throughout then gives

$$\hbar\frac{\partial\Lambda}{\partial t}\psi' + i\hbar\frac{\partial\psi'}{\partial t} = \left[\frac{1}{2m}\left[-\hbar(\boldsymbol{\nabla}\Lambda) - i\hbar\boldsymbol{\nabla} - q\mathbf{A}' + q(\boldsymbol{\nabla}f)\right]^2 + q\phi' + q\frac{\partial f}{\partial t}\right]\psi' \qquad \text{(3.9.1)}$$

-- If we now choose the arbitrary function $\Lambda(\mathbf{r},t)$ such that

$$\Lambda(\mathbf{r},t) = \frac{q}{\hbar}f(\mathbf{r},t)$$

then

$$\hbar(\boldsymbol{\nabla}\Lambda) = q(\boldsymbol{\nabla}f) \ ; \qquad \hbar\frac{\partial\Lambda}{\partial t}\psi' = q\frac{\partial f}{\partial t}\psi'$$

and all terms involving $f(\mathbf{r},t)$ or $\Lambda(\mathbf{r},t)$ in equation (3.9.1) cancel :

$$\boxed{i\hbar\frac{\partial\psi'}{\partial t} = \frac{1}{2m}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}'(\mathbf{r},t)\right]^2\psi' + q\phi'(\mathbf{r},t)\psi'} \qquad \text{(3.9.2)}$$

Gauge Invariance (6)

-- Equation (3.9.2) is now of the same form as the original Schrödinger equation (3.4.1), with (ϕ, $\mathbf{A}$, ψ) replaced by (ϕ', $\mathbf{A}'$, ψ')

Thus Schrödinger's equation for a charged particle in an EM field is invariant under a gauge transformation of the form

$$\boxed{\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla} f \;; \quad \phi \to \phi' = \phi - \frac{\partial f}{\partial t} \;; \quad \psi \to \psi' = \psi e^{i(q/\hbar) f}}$$

where $f(\mathbf{r},t)$ is an arbitrary function of position and time

-- Gauge invariance is of importance not just in electromagnetism, but more generally to the description of particle interactions in the Standard Model of particle physics :

$\rightarrow$ gauge invariance is promoted to a fundamental underlying symmetry principle which determines the form of the EM, weak, and strong interactions (including Maxwell's equations)

Gauge invariance : B = 0

-- A case of interest is the seemingly trivial example of a field-free region, with $\mathbf{B} = 0$ throughout

In this case, the simplest choice of gauge is just to take $\mathbf{A} = 0$ everywhere, but this is not the only possibility …

-- More generally, for a region where $\mathbf{B} = 0$, we can choose from a continuum of gauges with $\mathbf{A} \neq 0$ since, for any function $\chi(\mathbf{r})$, we have

$$\mathbf{A}(\mathbf{r}) = \boldsymbol{\nabla}\chi(\mathbf{r}) \quad \Rightarrow \quad \mathbf{B} = \boldsymbol{\nabla} \wedge \mathbf{A} = 0$$

Integrating from an arbitrary fixed point $\mathbf{r}_0$ along any choice of path to a point $\mathbf{r}$ then gives

$$\chi(\mathbf{r}) - \chi(\mathbf{r}_0) = \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s}$$

-- Applying a gauge transformation of the form on the previous slide, with the function f set to $f = -\chi$, produces

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla}(-\chi) = 0 \; ; \qquad \psi \to \psi' = \psi e^{-i(q/\hbar)\chi}$$

Gauge invariance : B = 0 (2)

-- Hence the wavefunction $\psi \equiv \psi_\chi$ in the gauge with $\mathbf{A} = \nabla\chi$, and the wavefunction $\psi' \equiv \psi_0$ in the gauge with $\mathbf{A} = 0$, are related as

$$\psi_0(\mathbf{r}) = \psi_\chi(\mathbf{r})e^{-i(q/\hbar)\chi(\mathbf{r})}$$

-- Inserting the integral form of the function $\chi(\mathbf{r})$, and absorbing the constant overall phase factor

$$e^{-i(q/\hbar)\chi(\mathbf{r}_0)}$$

into the wavefunction ψ_χ, the connection between wavefunctions in different gauges for a field-free region can be taken to be

$$\boxed{\psi_\chi(\mathbf{r}) = \psi_0(\mathbf{r}) \exp\left(i\frac{q}{\hbar}\int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s}\right)} \qquad \textbf{(3.12.1)}$$

The phase factor on the right-hand side above is independent of the choice of path from the (fixed, arbitrary) point $\mathbf{r}_0$ to the point $\mathbf{r}$

-- Equation (3.12.1) will prove useful in understanding the *Aharonov-Bohm effect* …

The Aharanov-Bohm Effect

-- In classical physics, it is the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$ that have physical significance

The potentials $\mathbf{A}$ and ϕ are just a mathematical convenience, and can be changed using a gauge transformation, with no observable effect

-- Quantum mechanics is different ; the vector potential $\mathbf{A}$ acquires physical significance ;

$\rightarrow$ changing $\mathbf{A}$ without changing $\mathbf{B}$ can lead to observable consequences

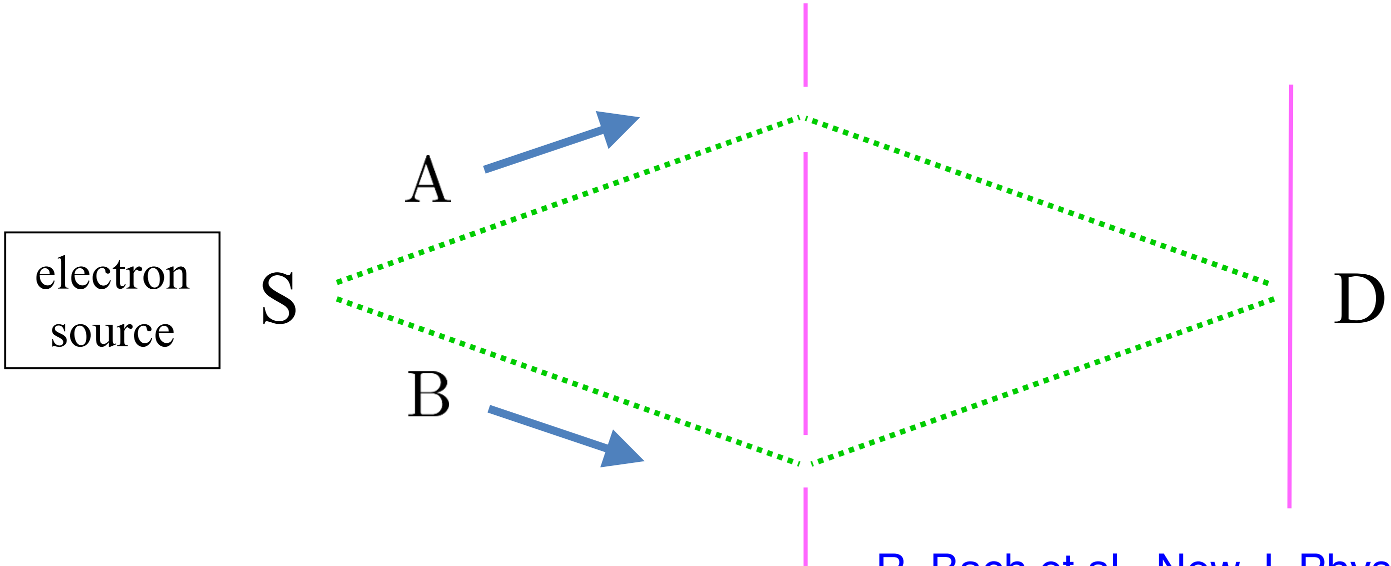
-- Aharanov and Bohm (1959) proposed demonstrating this by looking for interference effects using electrons in a double-slit set-up

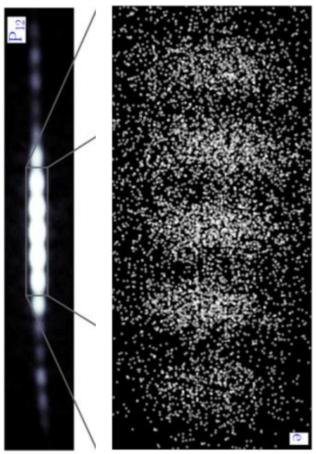
Y. Aharanov & D. Bohm, Phys. Rev. **115** (1959) 485

Their suggestion was subsequently confirmed experimentally, and goes by the name of the *Aharanov-Bohm effect*

The Aharanov-Bohm Effect (2)

-- Consider a standard double-slit arrangement, initially with zero magnetic field, $\mathbf{B} = 0$, everywhere :





R. Bach et al., New J. Phys. **15** (2013) 033018

-- A fringe pattern will be produced on the screen as a result of interference between contributions associated with the two possible paths A and B :

$$I \propto |\psi_{\rm D}|^2 = |\psi_{\rm A} + \psi_{\rm B}|^2$$

[a reasonable-looking expression which hides a can of worms – but if it works for optics it should work for quantum !]

The Aharanov-Bohm Effect (3)

-- For the gauge with $\mathbf{A} = 0$ everywhere, the wavefunction at a point D on the screen can be written as

$$\psi_{\mathrm{D},0} = \psi_{\mathrm{A},0} + \psi_{\mathrm{B},0} \qquad \textbf{(3.15.1)}$$

-- From equation (3.12.1), choosing $\mathbf{r}_0$ to be the source point S, the wave-function on the screen for a general gauge $\mathbf{A} = \nabla\chi$ is then given by

$$\psi_{\mathrm{D},\chi} = \psi_{\mathrm{A},0} \exp\left(i\frac{q}{\hbar}\int_{\mathrm{A}} \mathbf{A}(\mathbf{s})\cdot \mathrm{d}\mathbf{s}\right) + \psi_{\mathrm{B},0} \exp\left(i\frac{q}{\hbar}\int_{\mathrm{B}} \mathbf{A}(\mathbf{s})\cdot \mathrm{d}\mathbf{s}\right) \qquad \textbf{(3.15.2)}$$

-- The line integrals above are the same for paths A and B, as can be seen by applying the integral version of $\mathbf{B} = \boldsymbol{\nabla} \wedge \mathbf{A}$ to a clockwise loop :

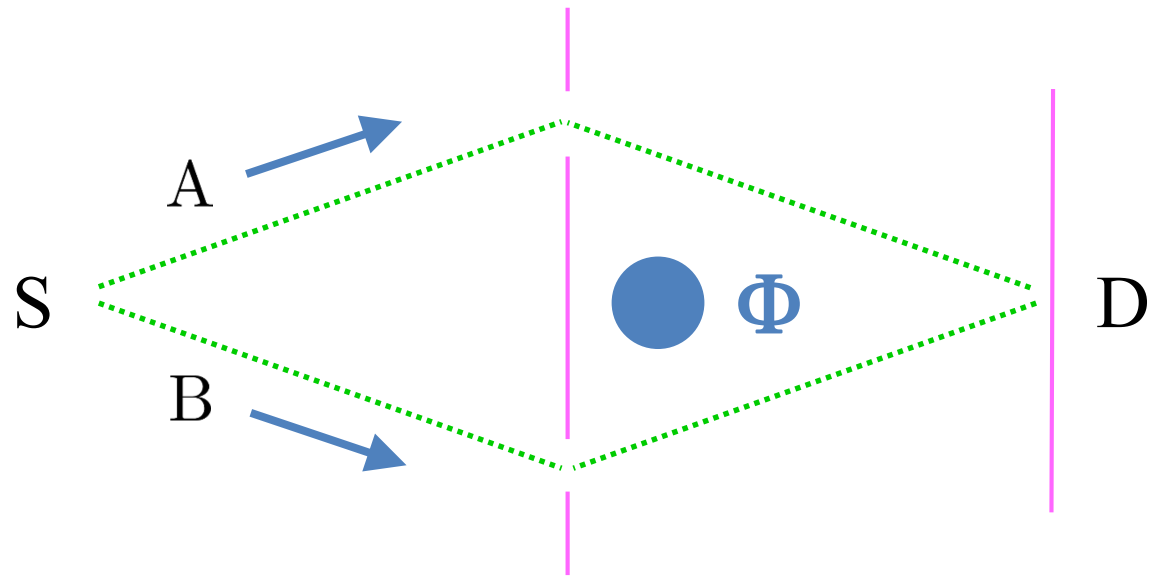
$$\oint \mathbf{A}(\mathbf{s})\cdot \mathrm{d}\mathbf{s} = \int_{\mathrm{A}} \mathbf{A}(\mathbf{s})\cdot \mathrm{d}\mathbf{s} - \int_{\mathrm{B}} \mathbf{A}(\mathbf{s})\cdot \mathrm{d}\mathbf{s} = \int_S \mathbf{B}(\mathbf{r})\cdot \mathrm{d}\mathbf{S} = 0$$

Hence the two phase factors in equation (3.15.2) are equal, and the inter-ference pattern on the screen is independent of the choice of gauge :

$$I \propto \left|\psi_{\mathrm{A},\chi} + \psi_{\mathrm{B},\chi}\right|^2 = \left|\psi_{\mathrm{A},0} + \psi_{\mathrm{B},0}\right|^2 \qquad \textbf{(3.15.3)}$$

The Aharanov-Bohm Effect (4)

-- Now place a solenoid carrying flux Φ (none of which can escape) directly behind the two slits :



The solenoid is shielded such that electrons cannot physically penetrate the solenoid region

-- If the magnetic flux Φ is contained entirely within the solenoid, then we still have $\mathbf{B} = 0$ everywhere outside the solenoid, and, in particular :

we still have $\mathbf{B} = 0$ at all points along the two trajectories A and B

The Aharanov-Bohm Effect (5)

-- However the vector potential $\mathbf{A}$ outside the solenoid must change :

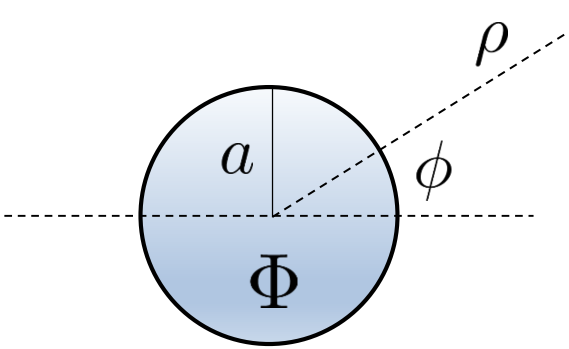
we *cannot* have $\mathbf{A} = 0$ at all points along the two trajectories A and B

This can be seen from the integral version of $\mathbf{B} = \boldsymbol{\nabla} \wedge \mathbf{A}$: the line integral of $\mathbf{A}$ around any closed loop enclosing the solenoid must be non-zero :

$$\oint \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s} = \int_S \mathbf{B}(\mathbf{r}) \cdot \mathrm{d}\mathbf{S} = \Phi \neq 0$$

-- e.g. in cylindrical polar coordinates (ρ,ϕ,z), the vector potential $\mathbf{A}$ in the region $\rho > a$ outside the solenoid can be taken to be

$$\mathbf{A} = (0, A_\phi, 0) \; ; \qquad A_\phi = \frac{\Phi}{2\pi\rho}$$



This is of the form

$$\mathbf{A}(\mathbf{r}) = \boldsymbol{\nabla}\chi(\mathbf{r}) \; ; \qquad \chi = \frac{\Phi\phi}{2\pi}$$

The function χ is *multiply-valued* under a full cycle $(\phi \to \phi + 2\pi)$

<u>*The Aharanov-Bohm Effect (6)*</u>

-- Since it is impossible to set $\mathbf{A}=0$ everywhere outside the solenoid, it would seem that equation (3.12.1) is inapplicable in this case
(as the wavefunction ψ_0 corresponding to the gauge $\mathbf{A}=0$ no longer exists)

-- In fact equation (3.12.1) <u>*can*</u> still be applied, but only to *separate* field-free regions containing *either* the path A alone, *or* the path B alone

[technically: the overall region outside the solenoid is *multiply connected*, while each separate trajectory lies within a *singly connected* region; equation (3.12.1) can be applied only within a singly connected region]

-- Thus, with the solenoid in place, the wavefunction at a point D on the screen can be written in a form which *looks* identical to the no-solenoid expression of equation (3.15.2) :

$$\psi_{\mathrm{D},\chi} = \psi_{\mathrm{A},0} \exp\left(i\frac{q}{\hbar}\int_{\mathrm{A}} \mathbf{A}(\mathbf{s})\cdot d\mathbf{s} \right) + \psi_{\mathrm{B},0} \exp\left(i\frac{q}{\hbar}\int_{\mathrm{B}} \mathbf{A}(\mathbf{s})\cdot d\mathbf{s} \right)$$

The Aharanov-Bohm Effect (7)

-- Now, however, the line integrals (and phases) above *cannot be equal* :

$$\int_{\mathrm{A}} \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s} - \int_{\mathrm{B}} \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s} = \oint \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s} = \Phi \neq 0$$

-- Extracting an overall common phase factor gives

$$\psi_{\mathrm{D},\chi} = \left[\psi_{\mathrm{A},0} \exp\left(i\frac{q}{\hbar}\Phi\right) + \psi_{\mathrm{B},0}\right] \exp\left(i\frac{q}{\hbar}\int_{\mathrm{B}} \mathbf{A}(\mathbf{s}) \cdot \mathrm{d}\mathbf{s}\right)$$

The intensity on the screen is therefore given by

$$\boxed{I \propto \left|\psi_{\mathrm{D},\chi}\right|^2 = \left|\psi_{\mathrm{A},0} \exp\left(i\frac{q}{\hbar}\Phi\right) + \psi_{\mathrm{B},0}\right|^2} \qquad \textbf{(3.19.1)}$$

-- The interference pattern is predicted to depend on the flux Φ contained within the solenoid

If the current in the solenoid is set to zero, or the solenoid is removed, so that $\Phi = 0$, we recover the original interference pattern of equation (3.15.3)

The Aharanov-Bohm Effect (8)

-- The dependence on Φ enters via a phase factor $e^{i\delta}$, where for electrons ($q = -e$), the phase angle δ is

$$\boxed{|\delta| = \frac{e\Phi}{\hbar} = 2\pi\frac{\Phi}{\Phi_0}}$$

$$\boxed{\Phi_0 \equiv \frac{h}{e} \approx 4.1 \times 10^{-15}\,\mathrm{T.m}^2}$$

Φ_0 is known as the *flux quantum*

-- Experimentally : the Aharanov-Bohm effect can be tested by comparing the interference patterns observed with the solenoid “on” and the solenoid “off”, while keeping all other parameters unchanged

The A-B Effect : experimental observation

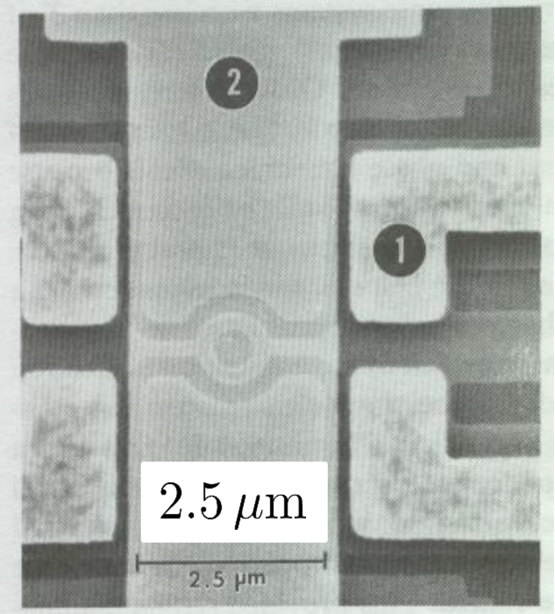
-- The first observation of the A-B effect is generally considered to be an experiment by Chambers (1960) R. G. Chambers, Phys. Rev. Lett. **5** (1960) 3

However residual doubts were expressed about possible systematic effects due to escaping flux

-- The first conclusive observation (1986) used a magnet covered with a superconducting layer (see the PtII E+O course)

A. Tonomura et al., Phys. Rev. Lett. **56** (1986) 792

-- Instead we choose a later example which used a micron-scale metal and GaAs/AlGaAs semiconductor ring structure :

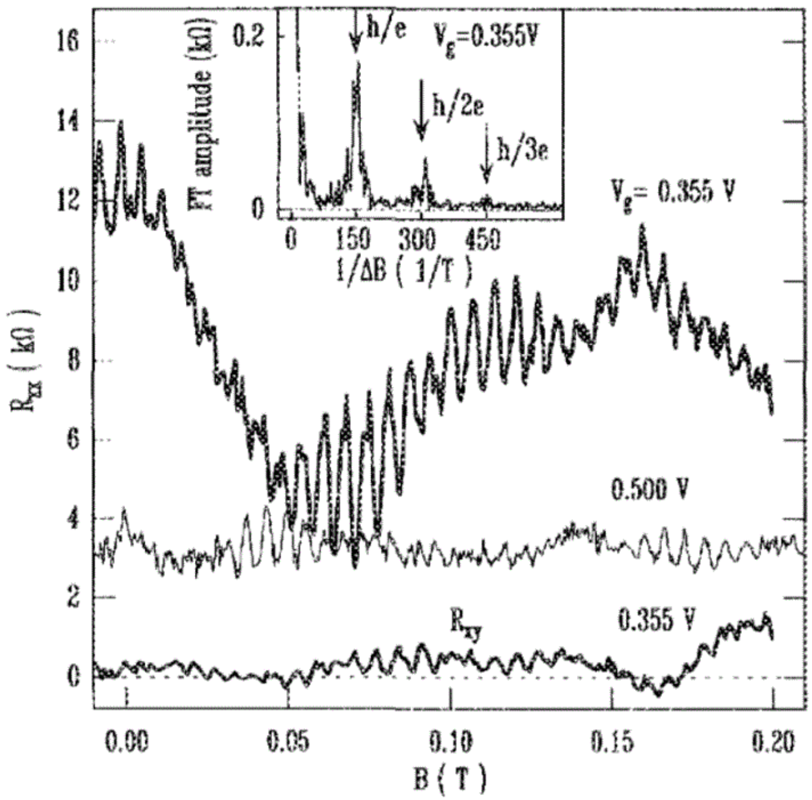


Cooled to a temperature $T \sim 25$ mK

K. Lee, .., **C. Ford** et al., Appl. Phys. Lett. **55** (1989) 625

The A-B Effect : experimental observation (2)

-- Large oscillations in resistance were observed as a function of the magnetic field strength B applied through the centre of the ring :



Inset : Fourier transform of data

(the peak at $h/2e$ is due to paths which encircle the ring twice)

up to $\pm\,40\%$ variations in R

-- At the time (1989), this was by far the clearest example of an A-B signal

[though the aim of the experiment was to use the A-B effect to demonstrate that the device was well manufactured, rather than to observe the A-B effect *per se*]

The Aharanov-Bohm Effect : Summary

-- In summary, in quantum physics, introducing the vector potential $\mathbf{A}$ is *essential*, not just a matter of mathematical convenience

-- Even when a particle moves through a region with no magnetic field ($\mathbf{B} = 0$ at all points along the particle's path), its quantum state acquires an extra phase which depends on $\mathbf{A}(\mathbf{r})$

This phase is normally unobservable, leaving $|\psi(\mathbf{r})|^2$ unchanged for all possible paths, but observable consequences can arise through interference effects (the Aharanov-Bohm effect)

-- In general, other (non-magnetic) contributions to the phase will also be present, potentially masking the A-B effect :

$\rightarrow$ the magnetic contribution (the A-B effect) can be isolated by varying the magnetic flux Φ, while keeping all other parameters constant

The Coulomb Gauge

-- Now return to the Hamiltonian of slide 3.4 describing a non-relativistic charged particle moving in an EM field :

$$\hat{H} = \frac{1}{2m}\left[\hat{\boldsymbol{p}} - q\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t)$$

-- Expanding out the first term explicitly, Schrödinger's equation can be written as

$$\hat{H}\psi = \frac{1}{2m}\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right]\cdot\left[-i\hbar\boldsymbol{\nabla} - q\mathbf{A}\right]\psi + q\phi\psi = i\hbar\frac{\partial\psi}{\partial t}$$

(3.24.1)

Using the identity

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

the Hamiltonian in equation (3.24.1) can be written as

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

(3.24.2)

The Coulomb gauge (2)

-- It is often convenient to work in a particular gauge, a common choice being the *Coulomb gauge*

$$\boxed{\boldsymbol{\nabla} \cdot \mathbf{A} = 0}$$

(observable quantities are independent of this choice)

The Coulomb gauge must always exist : to see this, suppose we are working initially in a gauge with

$$\boldsymbol{\nabla} \cdot \mathbf{A} \neq 0$$

Applying a gauge transformation

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla} f \ ; \qquad \boldsymbol{\nabla} \cdot \mathbf{A} \to \boldsymbol{\nabla} \cdot \mathbf{A}' = \boldsymbol{\nabla} \cdot \mathbf{A} + \nabla^2 f$$

with $f(\mathbf{r},t)$ chosen to be a solution of $\nabla^2 f = -(\boldsymbol{\nabla} \cdot \mathbf{A})$ then gives

$$\boldsymbol{\nabla} \cdot \mathbf{A}' = 0$$

-- In the Coulomb gauge, the Hamiltonian of equation (3.24.2) simplifies as

$$\boxed{\hat{H} = \frac{1}{2m}\left[-\hbar^2\nabla^2 + 2i\hbar q\,\mathbf{A} \cdot \boldsymbol{\nabla} + q^2\mathbf{A}^2\right] + q\phi} \qquad \textbf{(3.25.1)}$$

The symmetric gauge

-- If the magnetic field $\mathbf{B}$ is stationary and uniform, a convenient choice of Coulomb gauge is the *symmetric gauge*, defined by

$$\boxed{\mathbf{A}(\mathbf{r}) = -\frac{1}{2}\mathbf{r} \wedge \mathbf{B}} \qquad \textbf{(3.26.1)}$$

To check this is valid, orient the z-axis along the $\mathbf{B}$ field direction :

$$\mathbf{B} = (0, 0, B_z) \ ; \qquad \mathbf{A}(\mathbf{r}) = -\tfrac{1}{2}\mathbf{r} \wedge \mathbf{B} = \tfrac{1}{2}B_z(-y, x, 0)$$

For B_z constant, we then find, as required

$$\boldsymbol{\nabla} \wedge \mathbf{A} = \mathbf{B} \ ; \qquad \boldsymbol{\nabla} \cdot \mathbf{A} = 0$$

There is nothing special about the z direction, so equation (3.26.1) must be valid for any uniform magnetic field $\mathbf{B}$, oriented in any direction

-- In the symmetric gauge, and for $\mathbf{B}$ directed along z, the operator $\mathbf{A} \cdot \nabla$ in equation (3.25.1) is

$$\mathbf{A} \cdot \boldsymbol{\nabla} = \frac{1}{2}B_z\left(-y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}\right)$$

The symmetric gauge (2)

-- Comparing with

$$\hat{L}_z = (\hat{\boldsymbol{r}} \wedge \hat{\boldsymbol{p}})_z = -i\hbar\,(\hat{\boldsymbol{r}} \wedge \boldsymbol{\nabla})_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

and using $B_z\hat{L}_z = \mathbf{B}\cdot\hat{\boldsymbol{L}}$ then gives

$$\mathbf{A}\cdot\boldsymbol{\nabla} = \frac{i}{2\hbar}\mathbf{B}\cdot\hat{\boldsymbol{L}} \qquad (\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \wedge \hat{\boldsymbol{p}}) \qquad \textbf{(3.27.1)}$$

This must hold for *any* uniform $\mathbf{B}$, since the choice of z axis is arbitrary

-- In the symmetric gauge, the factor A^2 in equation (3.25.1) is

$$A^2 = \frac{1}{4}(\mathbf{r}\wedge\mathbf{B})^2 = \frac{1}{4}\left[r^2B^2 - (\mathbf{r}\cdot\mathbf{B})^2\right] \qquad \textbf{(3.27.2)}$$

-- Substituting from equations (3.27.1) and (3.27.2), the Hamiltonian (3.25.1) for a uniform magnetic field $\mathbf{B}$, in the symmetric gauge, is

$$\boxed{\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{q}{2m}(\hat{\boldsymbol{L}}\cdot\mathbf{B}) + \frac{q^2}{8m}\left[B^2r^2 - (\mathbf{B}\cdot\mathbf{r})^2\right] + q\phi(\mathbf{r})} \qquad \textbf{(3.27.3)}$$

The symmetric gauge (3)

-- For an electron confined within an atom, we can estimate

$$\langle \hat{L}_z \rangle \sim \hbar \; ; \qquad \langle r \rangle \sim a_0 \approx 0.5 \times 10^{-10}\,\mathrm{m}$$

-- Hence, for an atom in an external magnetic field $\mathbf{B}$, the ratio of quadratic and linear B-field terms in equation (3.27.3) is of order

$$\frac{e^2 B^2 a_0^2 / 8m_\mathrm{e}}{eB\hbar/2m_\mathrm{e}} = \frac{eBa_0^2}{4\hbar} \approx 1.1 \times 10^{-6} \times (B/\mathrm{T})$$

-- Hence, for atomic electrons ($q = -e$), we can often neglect the quadratic (B^2) terms in equation (3.27.3), leaving just the linear magnetic field term

$$\hat{H}_B = \frac{e}{2m_\mathrm{e}} \hat{\boldsymbol{L}} \cdot \mathbf{B}$$

For a hydrogen atom in an external magnetic field $\mathbf{B}$, for example, the Hamiltonian can be taken, to good approximation, to be

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} + \frac{e}{2m_\mathrm{e}} (\hat{\boldsymbol{L}} \cdot \mathbf{B})$$

Orbital magnetic moment

-- The $\boldsymbol{L} \cdot \mathbf{B}$ term in the Hamiltonian can be written as

$$\boxed{\hat{H} = -\hat{\boldsymbol{\mu}}_L \cdot \mathbf{B} \; ; \qquad \hat{\boldsymbol{\mu}}_L = \frac{q}{2m}\hat{\boldsymbol{L}} = \gamma_L \hat{\boldsymbol{L}}}$$

where $\boldsymbol{\mu}_L$ is the *orbital magnetic moment* operator, and

$$\gamma_L = \frac{q}{2m} \qquad \textbf{(3.29.1)}$$

is known as the *gyromagnetic ratio*

-- For an electron ($q = -e$), the orbital magnetic moment operator is

$$(\hat{\boldsymbol{\mu}}_L)_{\mathrm{e}} = -\frac{e}{2m_{\mathrm{e}}}\hat{\boldsymbol{L}} = -\frac{\mu_{\mathrm{B}}}{\hbar}\hat{\boldsymbol{L}}$$

where μ_{B} is the *Bohr magneton* :

$$\boxed{\mu_{\mathrm{B}} \equiv \frac{e\hbar}{2m_{\mathrm{e}}} \approx 9.28 \times 10^{-24}\,\mathrm{J\,T^{-1}} \approx 5.79 \times 10^{-5}\,\mathrm{eV\,T^{-1}}}$$

Spin and Magnetic Moments

-- We have not yet taken ***spin*** (intrinsic angular momentum) into account :

Particles (electrons, muons, quarks, protons, neutrons, nuclei, ..) possess an *intrinsic* (or *internal*) magnetic moment proportional to their spin :

$$\hat{\boldsymbol{\mu}}_S = \gamma_S \hat{\boldsymbol{S}}$$

-- The interaction of an intrinsic (spin) magnetic moment with an external magnetic field $\mathbf{B}$ has the same form as found above for $\boldsymbol{L}$:

$$\boxed{\hat{H}_B = -\hat{\boldsymbol{\mu}}_S \cdot \mathbf{B} = -\gamma_S \hat{\boldsymbol{S}} \cdot \mathbf{B}} \qquad \textbf{(3.30.1)}$$

Overall, the orbital and spin magnetic moments combine to give

$$\hat{H}_B = -\hat{\boldsymbol{\mu}}_L \cdot \mathbf{B} - \hat{\boldsymbol{\mu}}_S \cdot \mathbf{B} = -(\gamma_L \hat{\boldsymbol{L}} + \gamma_S \hat{\boldsymbol{S}}) \cdot \mathbf{B}$$

$$(\gamma_L = q/2m)$$

Particle magnetic moments : spin-half

-- Fundamental, pointlike, spin-half particles (electrons, muons, tau-leptons, and quarks) are described by a Lorentz invariant wave equation known as the *Dirac equation* (see later)

-- The Dirac equation predicts that such particles possess an intrinsic angular momentum $\hbar/2$, and predicts that their intrinsic magnetic moment is

$$\boxed{\hat{\boldsymbol{\mu}}_S = \frac{q}{m}\hat{\boldsymbol{S}} \,, \qquad \gamma_S = \frac{q}{m}}$$

Comparing with equation (3.29.1), this is a factor of two larger than would be expected based on the *orbital* magnetic dipole moment

(spin can be said to be "twice as effective" as orbital angular momentum)

-- For the electron ($q = -e$, $m = m_{\mathrm{e}}$), for example, the Dirac equation predicts an intrinsic magnetic moment given by

$$(\hat{\boldsymbol{\mu}}_S)_{\mathrm{e}} = -\frac{e}{m_{\mathrm{e}}}\hat{\boldsymbol{S}} = -2\frac{\mu_{\mathrm{B}}}{\hbar}\hat{\boldsymbol{S}} \;; \qquad \mu_{\mathrm{B}} \equiv \frac{e\hbar}{2m_{\mathrm{e}}}$$

Particle magnetic moments : spin-half (2)

-- In fact, the intrinsic (spin) magnetic moment of the electron is found to differ slightly (by ~ 0.1%) from the Dirac equation prediction :

$$(\hat{\boldsymbol{\mu}}_S)_\mathrm{e} \approx -(1.0012)\frac{e}{m_\mathrm{e}}\hat{\boldsymbol{S}} \approx -(2.0023)\frac{\mu_\mathrm{B}}{\hbar}\hat{\boldsymbol{S}}$$

-- This is allowed for by introducing the "*g-factor*", g_e , defined such that

$$(\hat{\boldsymbol{\mu}}_S)_\mathrm{e} = -\frac{e}{2m_\mathrm{e}}g_\mathrm{e}\hat{\boldsymbol{S}} = -g_\mathrm{e}\frac{\mu_\mathrm{B}}{\hbar}\hat{\boldsymbol{S}}\,; \qquad (\gamma_S)_\mathrm{e} = -g_\mathrm{e}\frac{\mu_\mathrm{B}}{\hbar}$$

where $g_\mathrm{e} \cong 2.0023$ (compared to the Dirac prediction $g_\mathrm{e} = 2$)

-- For an electron moving in a magnetic field $\mathbf{B}$, the overall (orbital plus spin) interaction can then be written in the general form

$$\boxed{\hat{H}_B = \frac{e}{2m_\mathrm{e}}(\hat{\boldsymbol{L}} + g_\mathrm{e}\hat{\boldsymbol{S}})\cdot\mathbf{B}}$$

Or equivalently : $$\hat{H}_B = \frac{\mu_\mathrm{B}}{\hbar}(\hat{\boldsymbol{L}} + g_\mathrm{e}\hat{\boldsymbol{S}})\cdot\mathbf{B}$$

The (scalar) magnetic moment

-- The magnetic moment of a particle or system can also be specified via its *scalar* magnetic moment μ

(μ is usually referred to simply as "*the* magnetic moment")

(μ is the quantity usually listed in data tables)

For a spin 1/2 particle, μ is defined via the "spin-up" state $|\uparrow\rangle$ as

$$\boxed{\mu \equiv \langle\uparrow|\hat{\mu}_z|\uparrow\rangle = \gamma_S \langle\uparrow|\hat{S}_z|\uparrow\rangle = \gamma_S \frac{\hbar}{2}}$$

-- For the electron, $\gamma_S = -g_e \mu_B/\hbar$, the scalar magnetic moment μ_e is thus

$$\mu_e = -\frac{g_e}{2}\mu_B$$

In the approximation $g_e = 2$ the electron's magnetic moment is simply

$$\mu_e = -\mu_B$$

(g_e is known to better than 1 part in 10^{12} : see below)

Spin Precession

-- Consider a particle of spin S moving in a magnetic field $\mathbf{B}$; the time evolution of the expectation values of S is given by Ehrenfest's theorem as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{S}}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{\boldsymbol{S}}]\rangle$$

The Hamiltonian of equation (3.27.3) commutes with S ; the only non-commuting contribution to H is the spin interaction of equation (3.30.1) :

$$\hat{H} = -\hat{\boldsymbol{\mu}}_S\cdot\mathbf{B} = -\gamma_S\hat{\boldsymbol{S}}\cdot\mathbf{B}$$

-- The x-component of the commutator $[H,S]$ above involves

$$[\mathbf{B}\cdot\hat{\boldsymbol{S}},\hat{S}_x] = B_y[\hat{S}_y,\hat{S}_x] + B_z[\hat{S}_z,\hat{S}_x]$$

[EXAMPLES SHEET]

$$= i\hbar(-B_y\hat{S}_z + B_z\hat{S}_y) = i\hbar(\hat{\boldsymbol{S}}\wedge\mathbf{B})_x$$

Similarly for y and z , so $\langle\hat{\boldsymbol{S}}\rangle = (\langle\hat{S}_x\rangle,\langle\hat{S}_y\rangle,\langle\hat{S}_z\rangle)$ satisfies

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{S}}\rangle = \gamma_S\langle\hat{\boldsymbol{S}}\rangle\wedge\mathbf{B}} \qquad \textbf{(3.34.1)}$$

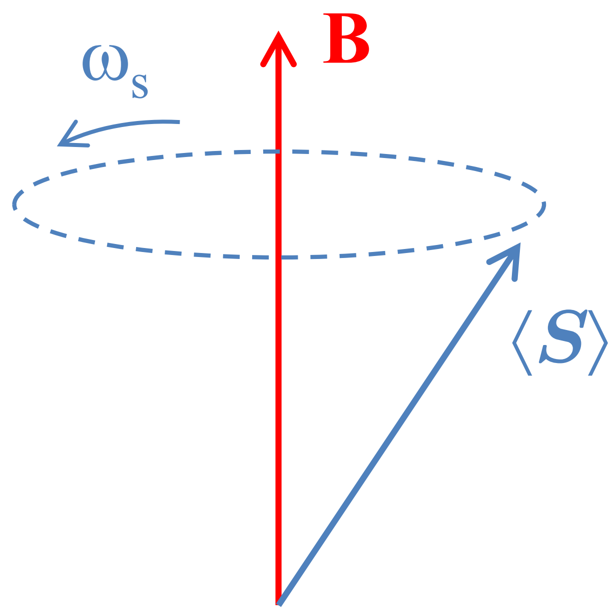
Spin precession (2)

-- The solutions of equation (3.34.1) correspond to *precession* of the three-vector $\langle \boldsymbol{S} \rangle$ of spin expectation values

$$\langle \hat{\boldsymbol{S}} \rangle = (\langle \hat{S}_x \rangle, \langle \hat{S}_y \rangle, \langle \hat{S}_z \rangle)$$

around $\mathbf{B}$, at the *Larmor frequency* ω_{s} :

$$\boxed{\omega_{\mathrm{s}} = \gamma_S B}$$



-- For example, for $\mathbf{B} = (0,0,B)$, equation (3.34.1) has solutions of the form

$$\langle \hat{S}_x \rangle = A \cos(\omega_{\mathrm{s}} t + \phi)\,; \qquad \langle \hat{S}_y \rangle = -A \sin(\omega_{\mathrm{s}} t + \phi)\,; \qquad \langle \hat{S}_z \rangle = \mathrm{constant}$$

-- Equation (3.34.1) can also be written as $\dfrac{\mathrm{d}}{\mathrm{d}t} \langle \hat{\boldsymbol{S}} \rangle = \langle \hat{\boldsymbol{\mu}}_S \rangle \wedge \mathbf{B}$

This is reminiscent of the equation $\dot{\mathbf{L}} = \mathbf{G} = \boldsymbol{\mu} \wedge \mathbf{B}$ which gives rise to precession in classical dynamics

Spin precession : spin-half

-- For a *spin-half* particle, the spin precession (Larmor) frequency is

$$\omega_{\mathrm{s}} = \gamma_S B = \frac{g}{2}\frac{qB}{m}$$

This can also be expressed as

$$\boxed{\omega_{\mathrm{s}} = \frac{g}{2}\omega_{\mathrm{c}}} \quad \text{where} \quad \boxed{\omega_{\mathrm{c}} \equiv \frac{qB}{m}} \quad \text{is the } \textit{cyclotron frequency}$$

ω_c is the frequency with which particles moving transverse to a magnetic field $\mathbf{B}$ undergo circular orbits $(mv^2/r = qvB\,; \quad v = r\omega_{\mathrm{c}})$

-- The difference between the spin and cyclotron (orbit) frequencies is

$$\boxed{\omega_{\mathrm{a}} \equiv \omega_{\mathrm{s}} - \omega_{\mathrm{c}} = \frac{g-2}{2}\frac{qB}{m}} \qquad \textbf{(3.36.1)}$$

Precision determinations of the muon magnetic moment are based on measuring the frequency difference ω_a (see below)

Spin precession : energy eigenstates

-- Orienting the z axis along the magnetic field $\mathbf{B}$, the Hamiltonian is

$$\mathbf{B} = (0, 0, B)\,; \qquad \hat{H} = -\gamma_S B \hat{S}_z$$

For a particle of spin s, the spin eigenstates $|sm_s\rangle$ defined with the z axis (the $\mathbf{B}$-field direction) as quantisation axis are also *energy* eigenstates :

$$\hat{S}_z |sm_s\rangle = m_s \hbar |sm_s\rangle$$

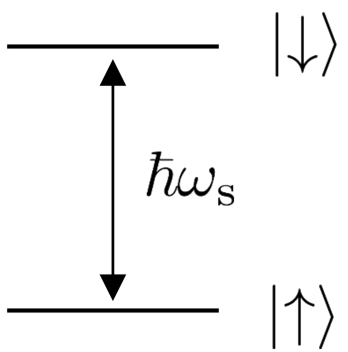
$$\Rightarrow \quad \hat{H}|sm_s\rangle = E_{m_s}|sm_s\rangle\,; \qquad E_{m_s} = -\gamma_S B m_s \hbar = -m_s \hbar \omega_{\mathrm{s}}$$

where ω_s is the Larmor frequency again : $\omega_{\mathrm{s}} = \gamma_S B$

-- Thus, in a magnetic field, for spin s, we obtain a set of $2s+1$ equally spaced energy levels, with energy spacing

$$\Delta E = \hbar\omega_{\mathrm{s}} = \hbar\gamma_S B$$

e.g. for $s = 1/2$:



e.g. for a $g = 2$ electron in $B = 1\ \mathrm{T}$:

$$\Delta E = \frac{\hbar e B}{m_{\mathrm{e}}} \approx 1.2 \times 10^{-4}\,\mathrm{eV}$$

Spin precession : wavefunction evolution

-- For a particle which is initially in a spin eigenstate, $|\psi(0)\rangle = |sm_s\rangle$, the spin state $|\psi(t)\rangle$ evolves as

$$|\psi(t)\rangle = \exp(-iE_{m_s}t/\hbar)\,|sm_s\rangle = \exp(im_s\omega_s t)\,|sm_s\rangle$$

The particle therefore remains in the state $|sm_s\rangle$ at all times

-- The expectation value of the spin z-component for the state $|\psi(t)\rangle$ is

$$\langle\psi(t)|\hat{S}_z|\psi(t)\rangle = \langle sm_s|\hat{S}_z|sm_s\rangle = m_s\hbar$$

The expectation values of the x and y components *vanish*, as is easily seen by introducing the ladder operators S_+ and S_- :

$$\langle\psi(t)|\hat{S}_{x,y}|\psi(t)\rangle \propto \langle sm_s|(\hat{S}_+ \pm \hat{S}_-)|sm_s\rangle = 0$$

-- Thus, for an initial spin state $|\psi(0)\rangle = |sm_s\rangle$, the vector of spin expectation values remains constant, and directed along z :

$$\boxed{\langle\psi(t)|\hat{\boldsymbol{S}}|\psi(t)\rangle = \langle sm_s|\hat{\boldsymbol{S}}|sm_s\rangle = (0, 0, m_s\hbar)} \qquad \textbf{(3.38.1)}$$

(a special case, with no "visible" precession)

Spin precession : wavefunction evolution (2)

-- Now generalise to an arbitrary initial spin state :

$$|\psi(0)\rangle = \sum_{m_s} c_{m_s} |sm_s\rangle$$

In this case, the state $|\psi\rangle$ evolves with time as

$$|\psi(t)\rangle = \sum_{m_s} c_{m_s} \exp(im_s\omega_{\mathrm{s}}t)|sm_s\rangle$$

-- The spin expectation values are now given by

$$\langle\psi(t)|\hat{\boldsymbol{S}}|\psi(t)\rangle = \sum_{m'_s, m_s} c^*_{m'_s} c_{m_s} \exp\left(i(m_s - m'_s)\omega_{\mathrm{s}}t\right)\langle sm'_s|\hat{\boldsymbol{S}}|sm_s\rangle$$

The x and y components $\langle S_x\rangle$, $\langle S_y\rangle$ involve matrix elements of the form

$$\langle sm'_s|\hat{S}_{x,y}|sm_s\rangle \propto \langle sm'_s|(\hat{S}_+ \pm \hat{S}_-)|sm_s\rangle$$

These matrix elements are non-zero only for $(m_s - m'_s) = \pm 1,$ giving a time dependence

$$e^{i(m_s - m'_s)\omega_{\mathrm{s}}t} = e^{\pm i\omega_{\mathrm{s}}t} \qquad (\omega_{\mathrm{s}} = \gamma_S B)$$

Spin precession : wavefunction evolution (3)

-- Hence $\langle S_x \rangle$ and $\langle S_y \rangle$ oscillate at the Larmor frequency ω_s, as already found using Ehrenfest's theorem (slide 3.35) :

$$\boxed{\langle \hat{S}_{x,y} \rangle = A_{x,y} \cos \omega_s t + B_{x,y} \sin \omega_s t}$$

-- For z, the matrix elements are non-zero only for $m'_s = m_s$:

$$\langle s m'_s | \hat{S}_z | s m_s \rangle = \delta_{m'_s, m_s} m_s \hbar$$

Thus $\langle S_z \rangle$ is constant (time-independent), also as found on slide 3.35 :

$$\boxed{\langle \hat{S}_z \rangle = \langle \psi(t) | \hat{S}_z | \psi(t) \rangle = \sum_{m_s} |c_{m_s}|^2 m_s \hbar = \text{constant}} \quad \textbf{(3.40.1)}$$

-- Thus, we again find that the vector $\langle \hat{\boldsymbol{S}} \rangle = \langle \psi(t) | \hat{\boldsymbol{S}} | \psi(t) \rangle$ of spin expectation values precesses about the magnetic field direction at the Larmor frequency $\omega_s = \gamma_S B$

Magnetic moments : the electron

-- The *electron* magnetic moment has been measured (Harvard, 2008) with a relative precision better than 1 part in 10^{12} :

$$(g_e/2)_{\text{expt}} = 1.00115965218073(28)$$

D. Hanneke et al., Phys. Rev. A 83 (2011) 052122

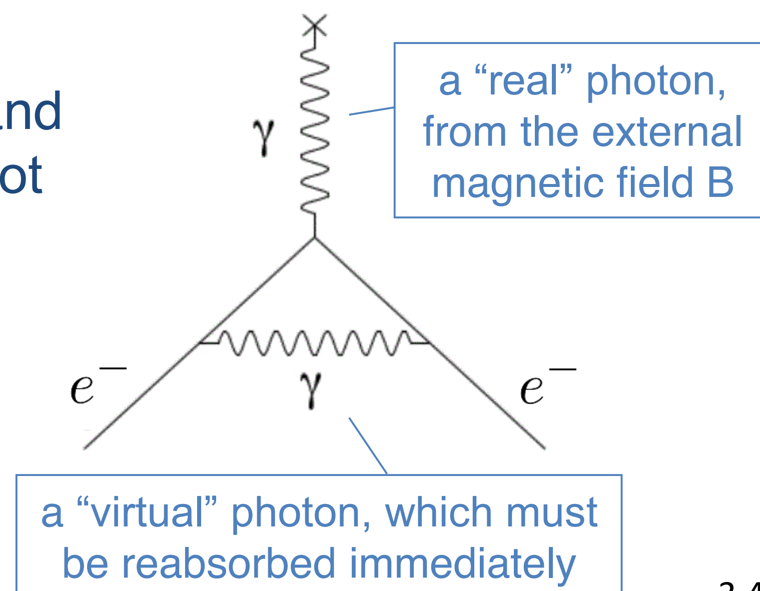
-- The small (~ 0.1%) deviation from $g_e = 2$ is resolved by *Quantum Electro-dynamics* (QED)

(the quantum theory of the electromagnetic field : more later)

-- *Very roughly* :

- In QED, the electron continually emits and reabsorbs "virtual" photons, which cannot escape as free particles

- The electron is not truly a single particle, but is effectively surrounded by a cloud of virtual photons, virtual electrons, virtual positrons, …



Magnetic moments : the electron (2)

-- QED perturbation theory calculations predict the magnetic moment as a power series in the *fine structure constant* $\alpha \cong 1/137$:

$$g_{\mathrm{e}} = 2 + g^{(1)}\left(\frac{\alpha}{\pi}\right) + g^{(2)}\left(\frac{\alpha}{\pi}\right)^2 + \ldots + g^{(5)}\left(\frac{\alpha}{\pi}\right)^5 + \ldots \qquad \textbf{(3.42.1)}$$

$$\left(g^{(1)} = 1.0, \quad g^{(2)} \approx -0.66, \quad g^{(3)} \approx 2.4, \quad g^{(4)} \approx -3.8, \quad g^{(5)} \approx 15.6 \right)$$

T. Aoyama, T. Kinoshita & M. Nio, Atom **7** (2019) 28

where

$$\boxed{\alpha \equiv \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137.036} \approx \frac{1}{137}}$$

-- An interferometer experiment using cesium-133 atoms recently (2018) improved the precision on the measured value of α by a factor ~3 :

$$1/\alpha = 137.035999046(27)$$

R. Parker et al., Science **360** (2018) 191

Using this value in equation (3.42.1) then gives a QED prediction for g_{e} with a precision similar to experiment :

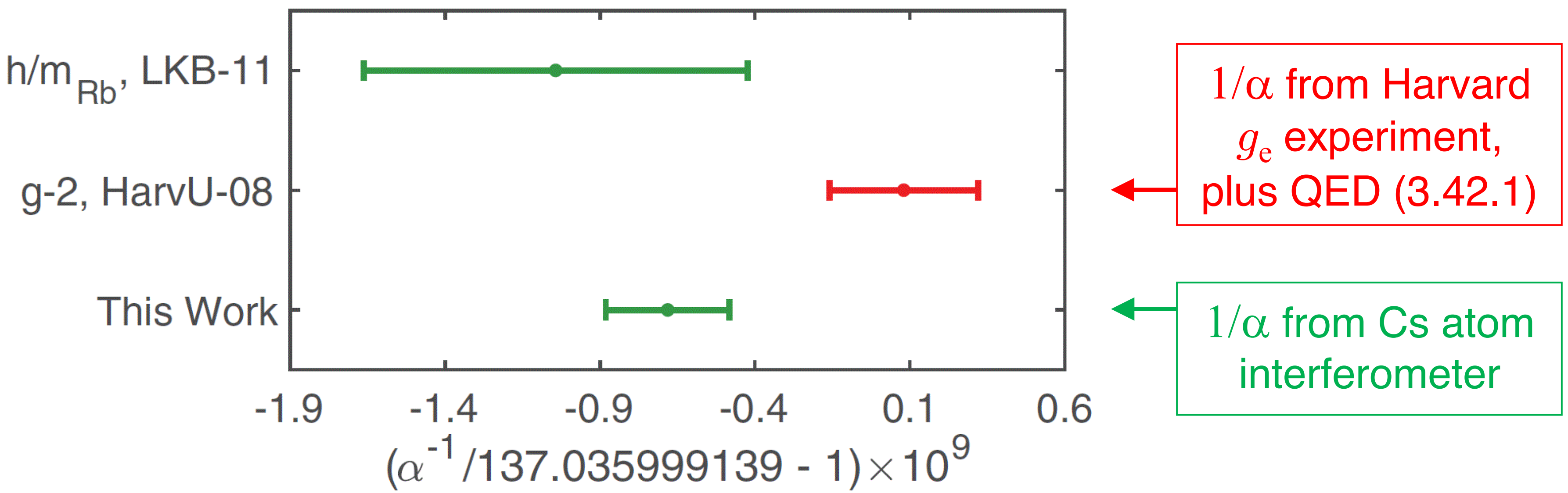
$$(g_{\mathrm{e}}/2)_{\mathrm{QED}} = 1.00115965218161(23)$$

Magnetic moments : the electron (3)

-- The QED prediction for g_e agrees with the measured value, albeit with a small (2.4 standard deviation) discrepancy

This is displayed below by inverting equation (3.42.1) to extract the value of $1/\alpha$ corresponding to the Harvard measurement of g_e :

R. Parker et al., Science 360 (2018) 191



-- Modulo this small discrepancy :

Quantum Mechanics (QED) works to better than 12 decimal places!

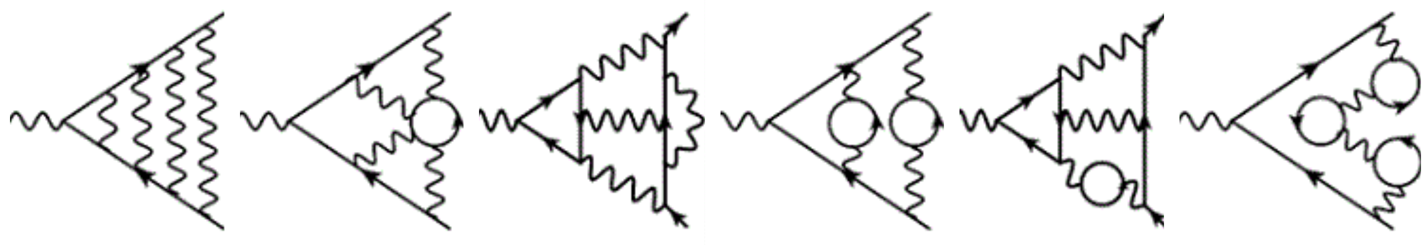
Magnetic moments : the electron (4)

-- The QED perturbation theory calculations (up to 5th order) are fiendishly difficult; they have taken many decades and are still not finalised

e.g. a new (2019) independent calculation of $g^{(5)}$ which disagrees slightly with the only other existing calculation

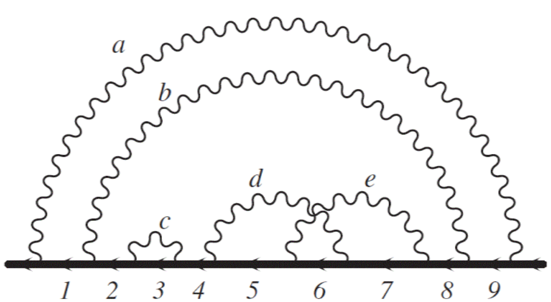
S. Volkov, arXiv:1909.08015 (Sept. 2019)

-- Some representative 4th-order Feynman diagrams (891 diagrams in total) :



P. Marquard et al., arXiv:1708.07138 (2017)

-- An example of a 5th-order diagram :



Each Feynman diagram represents a complex, multi-dimensional integral

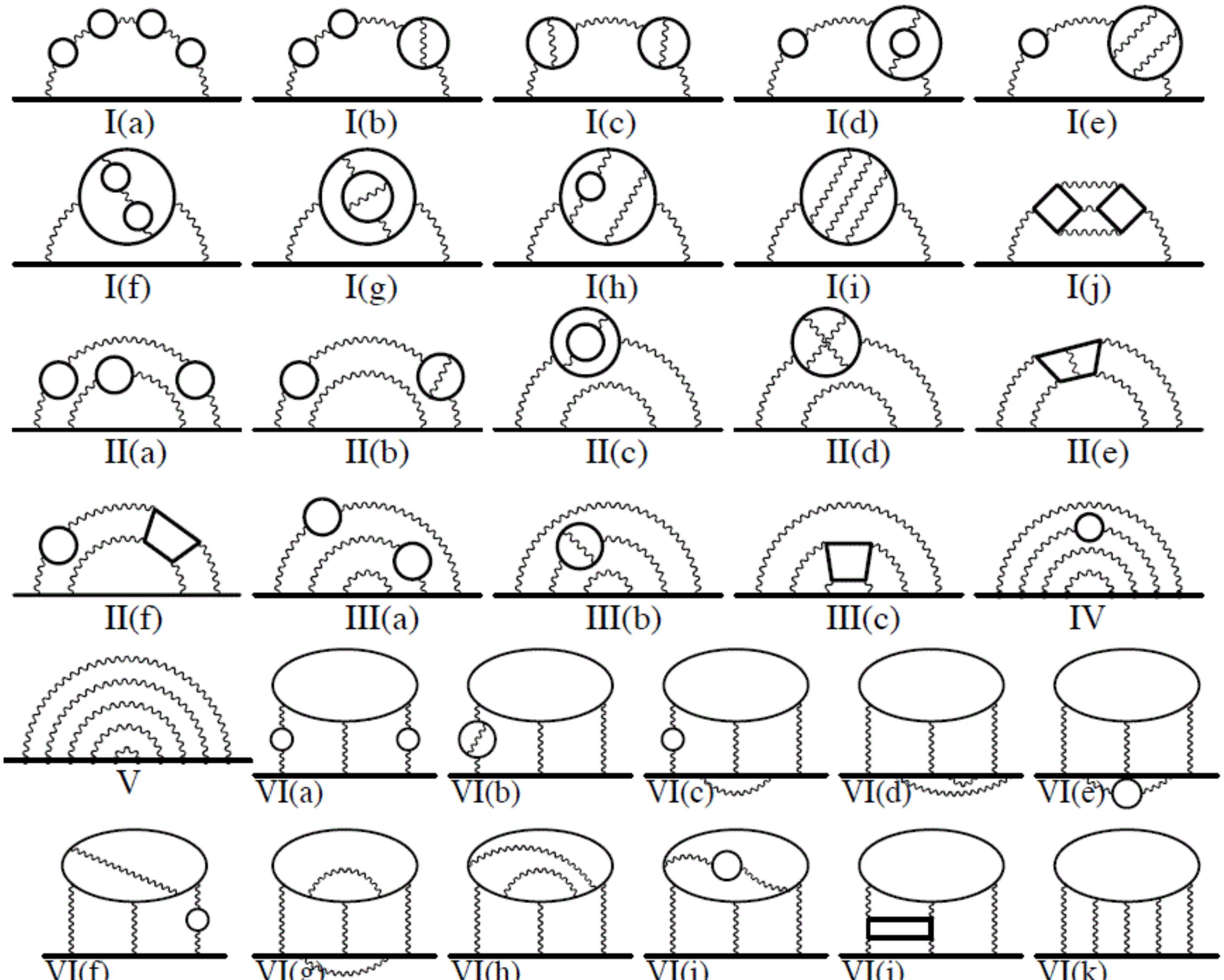
(numerical calculations maintain several thousand decimal places throughout)

T. Aoyama et al., Phys. Rev. D **96** (2017) 019901

Magnetic moments : the electron (5)

-- The 5th order diagrams (12672 diagrams in total, in 32 classes) :

T. Aoyama, T. Kinoshita & M. Nio, Atom **7** (2019) 28



Magnetic moments : the muon

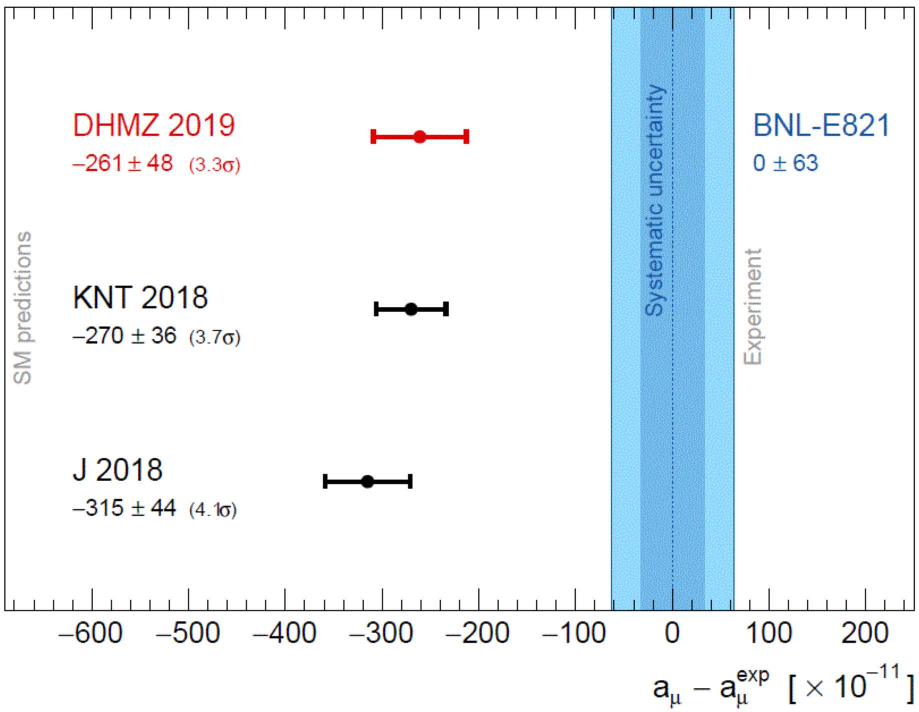
-- Now consider the *muon* : a heavy ($m_\mu / m_e = 206.77$), unstable (average rest-frame lifetime $\tau_\mu = 2.2\ \mu s$) version of the electron

There is currently a ~3.5σ discrepancy between measurement and QED :

theory

experiment

M. Davier et al., arXiv:1908.00921



$$a_\mu \equiv \frac{g_\mu - 2}{2}$$

(parts in 10^{11})

-- The quantity a_μ is known as the *anomalous magnetic moment*

Magnetic moments : the muon (2)

-- Theory and experiment have similar precision (better than 1 part in 10^9) :

Theory (DHMZ19) : $(g_\mu/2)_{\mathrm{QED}} = 1.00116591829(48)$

[M. Davier et al., arXiv:1908.00921 (July 2019)]

Experiment (E821) : $(g_\mu/2)_{\mathrm{expt}} = 1.00116592091(63)$

[G. W. Bennett et al., Phys. Rev. D **73** (2006) 072003]

The g-factor g_μ above is specified in terms of the *"muon magneton"* :

$$\mu_{\mathrm{B}}^{(\mu)} \equiv \frac{e\hbar}{2m_\mu} = \frac{m_{\mathrm{e}}}{m_\mu}\mu_{\mathrm{B}} \approx \frac{\mu_{\mathrm{B}}}{207}$$

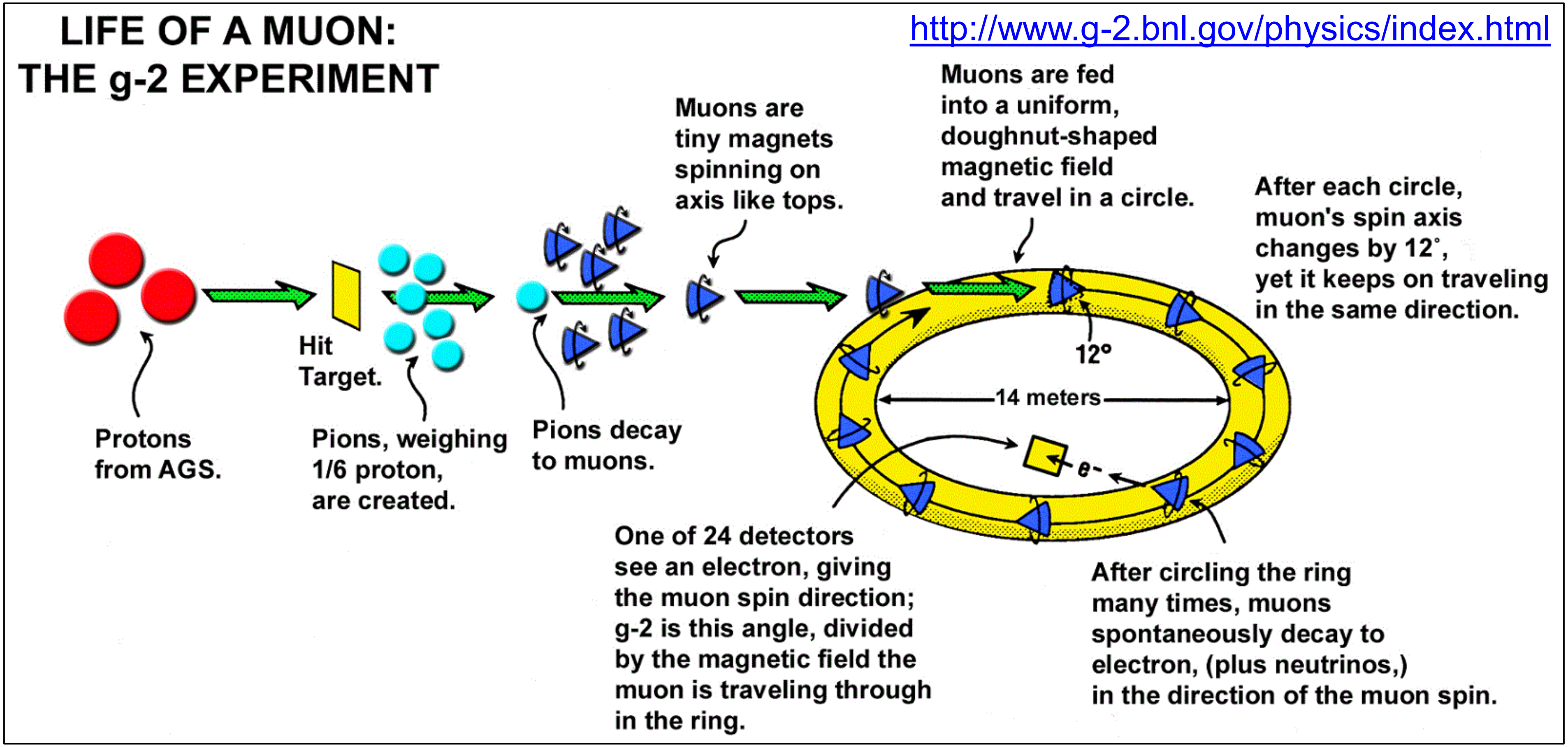
-- The discrepancy between QED and experiment may or may not need "new physics" to be resolved :

$\rightarrow$ new experiments and improved theoretical calculations are underway

So **if** the central values remain unchanged, the discrepancy between experiment and theory will grow to over 7 standard deviations by 2021

Magnetic moments : the muon (3)

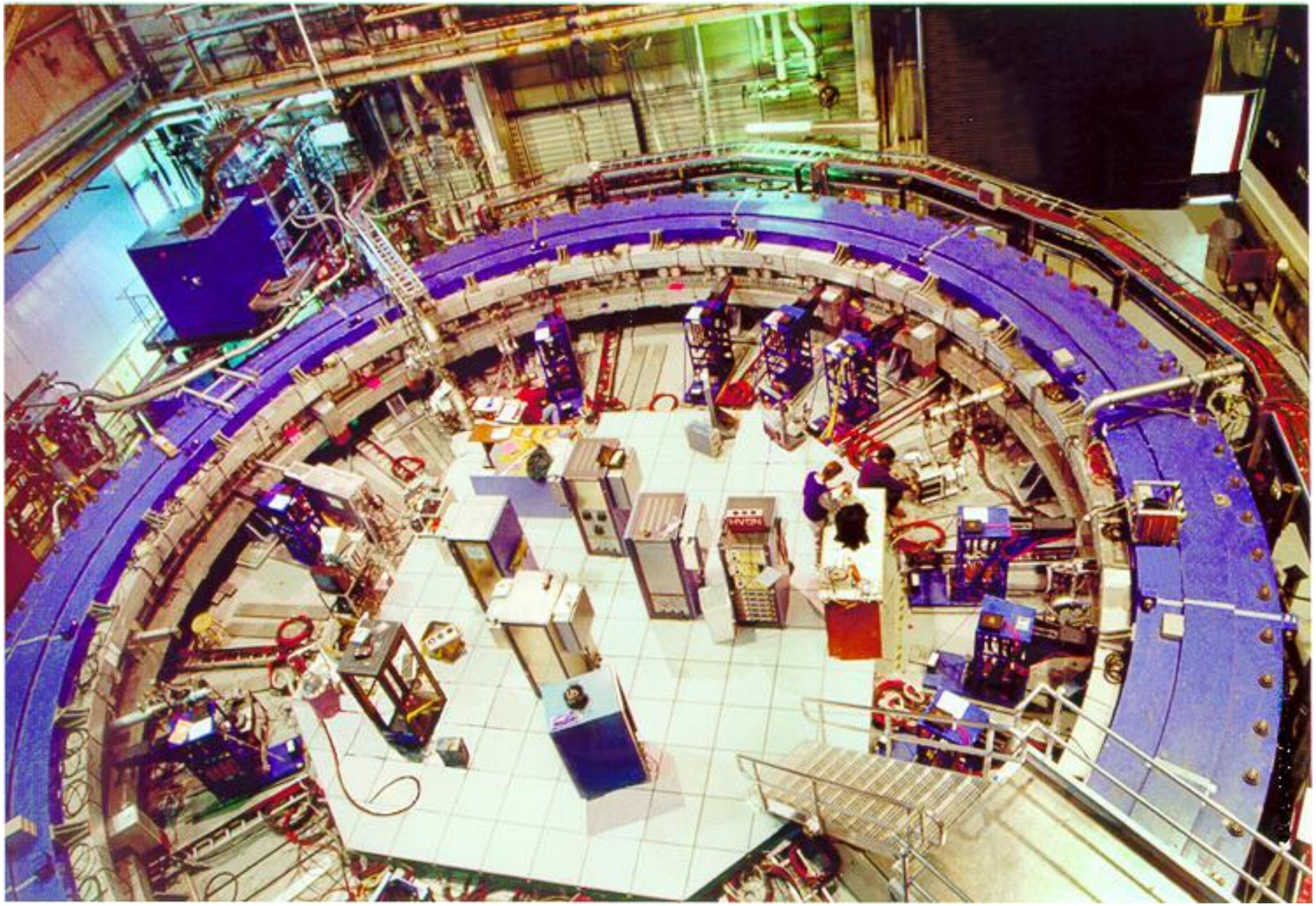
-- The experimental technique used to measure the muon magnetic moment is a beautiful example of spin precession in action ….



The same technique has been used in a series of experiments beginning at CERN in 1960 and culminating with E821 in Brookhaven, Long Island (2006)

Magnetic moments : the muon (4)

-- The E821 experiment (Brookhaven) :



http://www.g-2.bnl.gov/pictures/index.html

Magnetic moments : the muon (5)

-- In E821, relativistic muons ($v/c = 0.99941$) travel in a circular orbit around a ring containing a highly uniform (~ 1 ppm) magnetic field ($B = 1.4513$ T)

$\rightarrow$ the muon 3-mom. precesses at the cyclotron frequency $\omega_\mathrm{c} \equiv eB/m_\mathrm{e}$

-- The ring is initially ($t = 0$) filled with polarised muons, with the muon spin vector oriented along the muon momentum direction

-- Equation (3.36.1) for the difference, $\omega_\mathrm{a} = \omega_\mathrm{s} - \omega_\mathrm{c}$, between the spin and cyclotron precession frequencies,

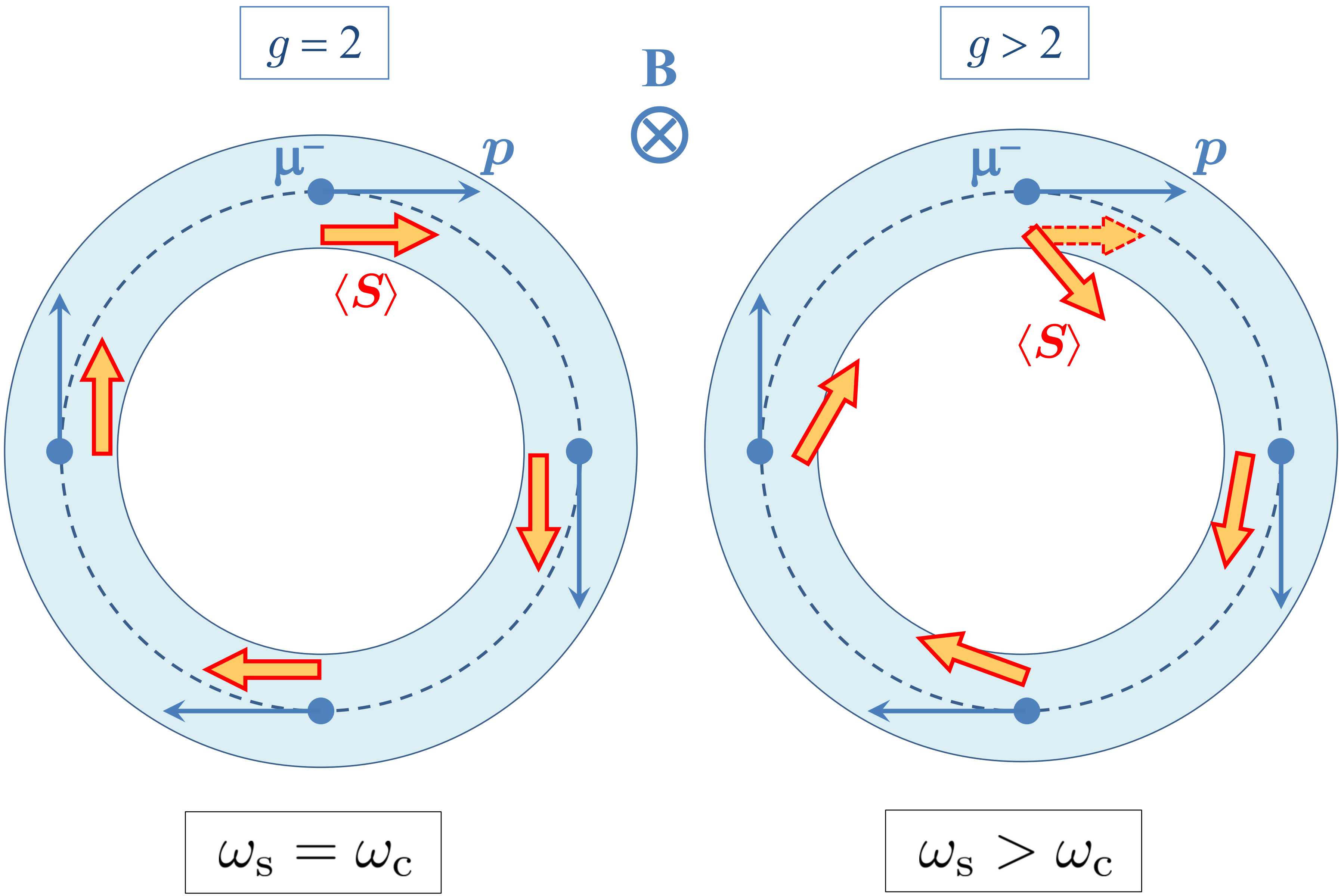
$$\boxed{\omega_\mathrm{a} = \frac{g-2}{2}\frac{qB}{m}} \qquad \textbf{(3.50.1)}$$

in fact holds also for *relativistic* particles

-- For $g = 2$, the spin and cyclotron frequencies are equal : $\omega_\mathrm{a} = 0$, $\omega_\mathrm{s} = \omega_\mathrm{c}$

$\rightarrow$ the muon spin vector would remain aligned with the muon momentum direction for all times $t > 0$

Magnetic moments : the muon (6)



Magnetic moments : the muon (7)

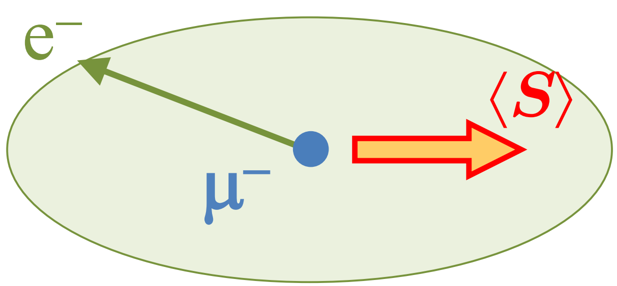
-- But for $g \approx 2.0023$, the muon spin $\langle \boldsymbol{S} \rangle$ precesses (slightly) *faster* than the muon momentum vector

$\rightarrow$ on each orbit, the spin direction $\langle \boldsymbol{S} \rangle$ rotates through an angle slightly ($\sim 12^{\mathrm{o}}$) greater than the muon momentum rotation angle (360^{o})

-- As they orbit, the muons decay to electrons (and neutrinos) :

$$\mu^- \rightarrow \mathrm{e}^- + \overline{\nu}_{\mathrm{e}} + \nu_\mu$$

In the muon rest frame, the electrons are emitted with a range of energies and a <u>*non-isotropic*</u> *angular distribution about the muon* ***spin*** *direction :*

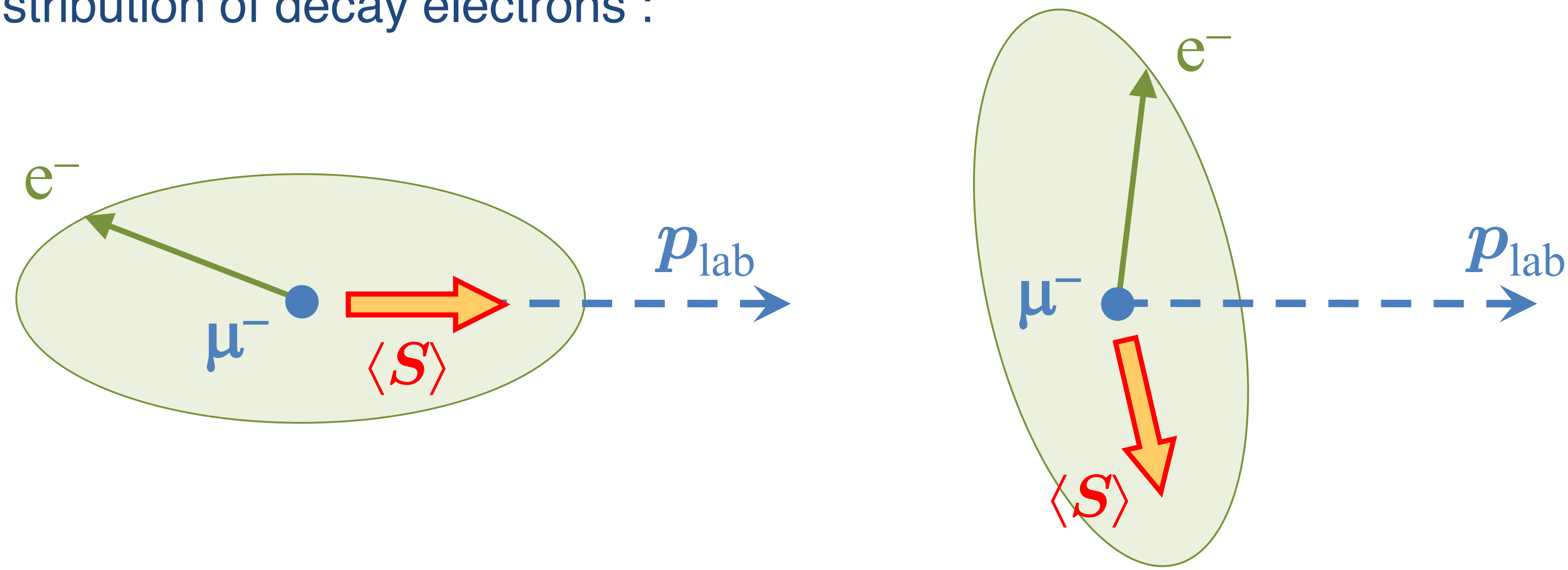


In a particle's rest frame, $\mathbf{p} \equiv 0$, the only quantity which can possibly introduce a preferred spatial direction is the ***spin***

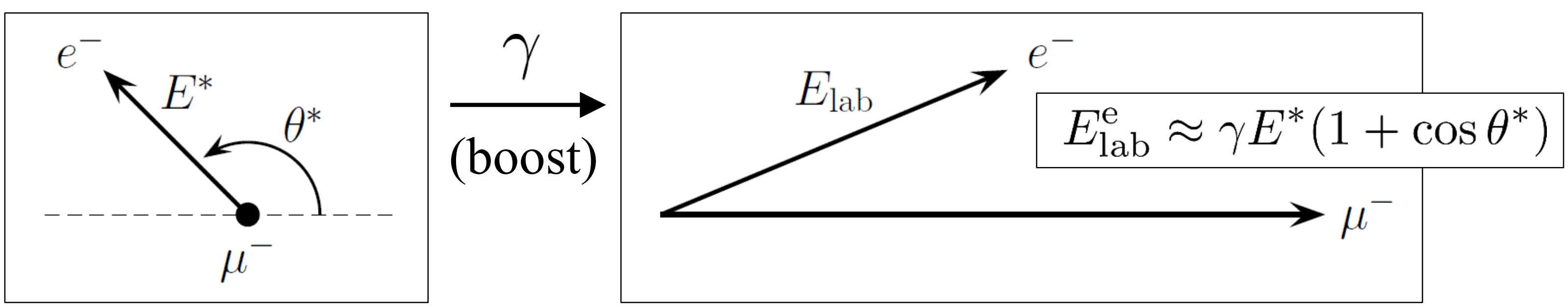
[Highly schematic : the angular distribution is not really elliptical.
In fact it is not even symmetric; due to *parity violation*, electrons are emitted preferentially in directions *opposite* to the muon spin direction]

Magnetic moments : the muon (8)

-- As the spin vector $\langle \boldsymbol{S} \rangle$ rotates about the muon direction, so too does the distribution of decay electrons :



-- Hence, after a Lorentz transformation to the lab frame …

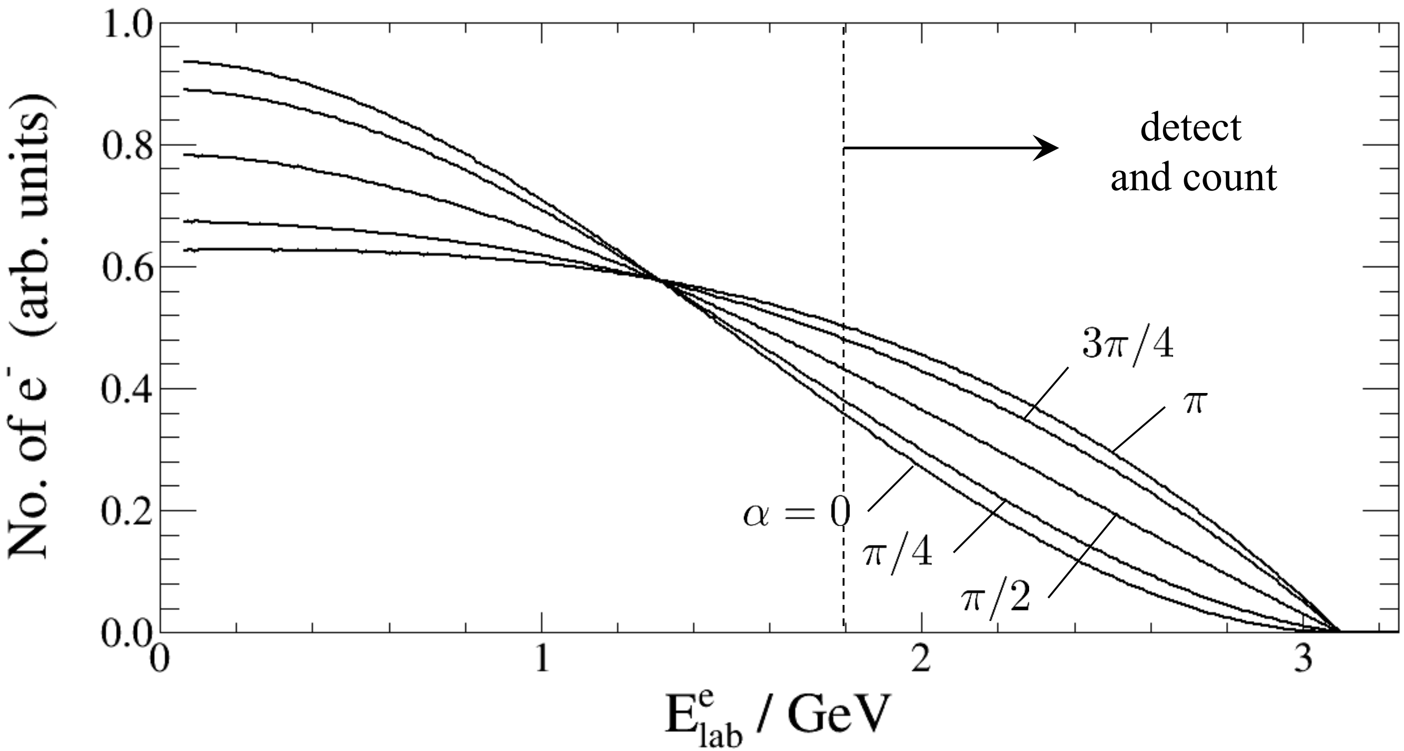


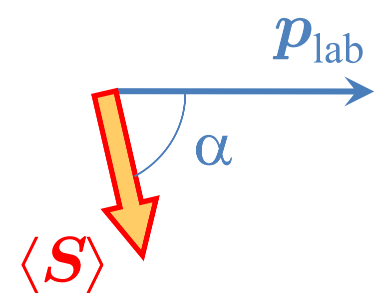
muon rest frame

lab frame

Magnetic moments : the muon (9)

… the distribution of electron energy in the lab frame depends on the angle between the spin and the boost (muon momentum) directions :





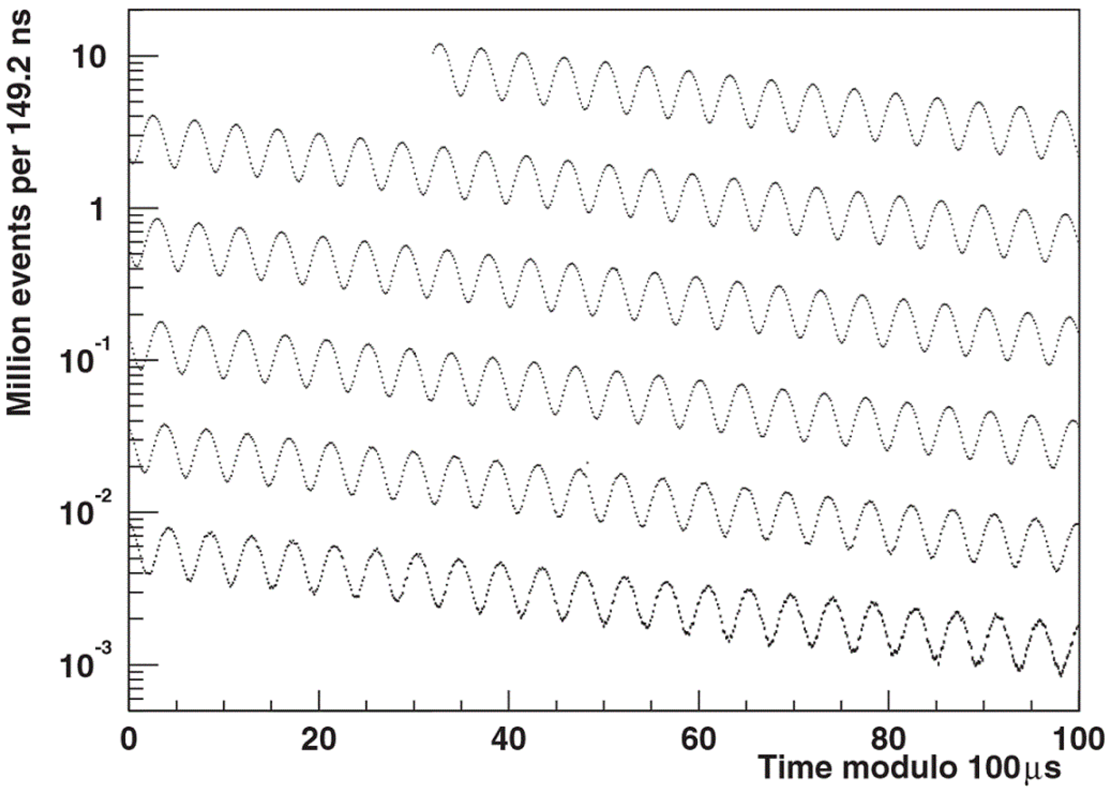
-- Electrons above a certain lab frame energy are detected and counted :

$\rightarrow$ the number of electrons detected varies as the spin $\langle \boldsymbol{S} \rangle$ rotates relative to the momentum $\boldsymbol{p}$ …

Magnetic moments : the muon (10)

-- Thus the number of electrons detected varies with time, with a periodic structure corresponding to the frequency ω_a with which the spin $\langle \boldsymbol{S} \rangle$ rotates relative to the momentum $\boldsymbol{p}$ …

G. W. Bennett et al., Phys. Rev. D **73** (2006) 072003



The plot contains $\sim 3 \times 10^9$ muon decays, about 40% of the total E821 data set

The periodic structure is super-imposed on a steady exponential fall due to the muon decay :

$$N_{\rm e}(t) = N_0 e^{-t/\tau}$$

(the muon has a mean lifetime of $\tau = 2.2\ \mu\text{s}$ in its rest frame)

Magnetic moments : the muon (11)

-- The periodic structure directly measures the difference ω_a between the cyclotron and spin precession frequencies

Rearranging equation (3.50.1) then determines a_μ, and hence g_μ, as

$$a_\mu \equiv \frac{g_\mu - 2}{2} = \frac{m\omega_{\mathrm{a}}}{eB}$$

-- The magnetic field $\mathbf{B}$ is calibrated and monitored by continually measuring the precession frequency ω_p for protons at rest in the same field

(using NMR probes: see later)

This allows a_μ to be determined from the well-measured quantity

$$\mathcal{R} = \frac{\omega_{\mathrm{a}}}{\omega_{\mathrm{p}}}$$

[EXAMPLES SHEET]

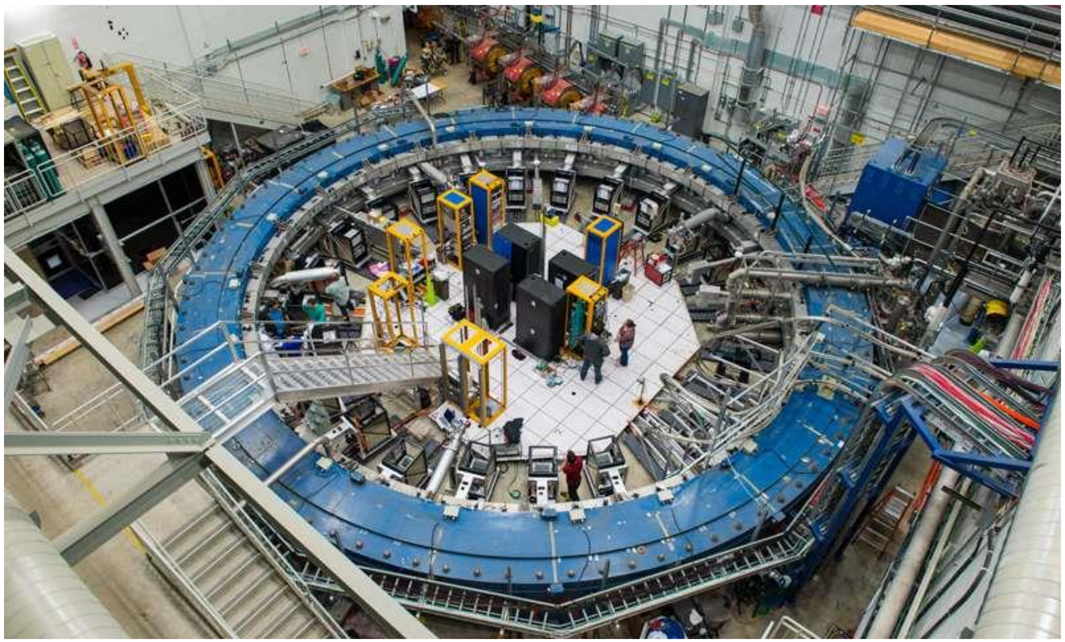
thereby avoiding the need to know the value of B explicitly

-- E821 determined a_μ with a precision of 0.5 ppm, and g_μ with a precision of 0.6 ppb (slide 3.47)

Magnetic moments : the muon (12)

A successor experiment to E821 (E989) is now underway at Fermilab, Chicago

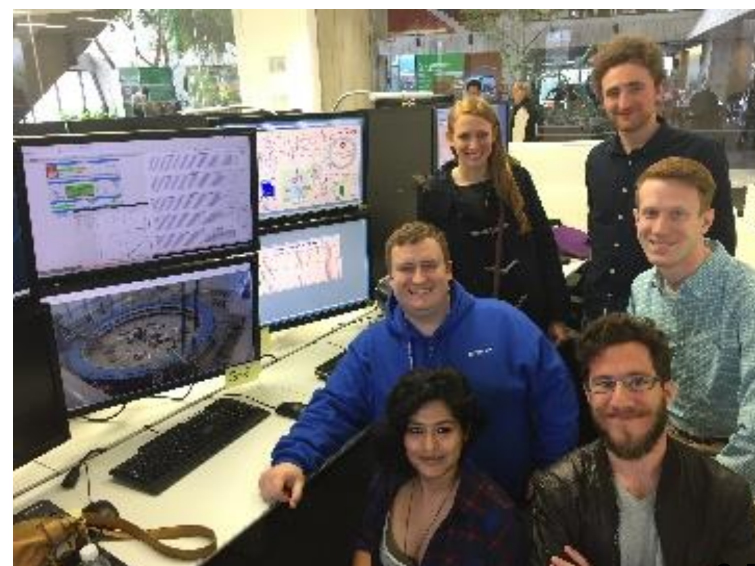
http://muon-g-2.fnal.gov/



→ projected to improve the experimental precision by a factor ~ 4 by 2020

Plus: experiment E34 at J-PARC (Japan), using a new technique: http://g-2.kek.jp/

E821 → E989
Long Island → Chicago



Magnetic moments : p, n, nuclei

-- For the proton ($q = +e$, $m = m_{\rm p}$) and neutron ($q = 0$), by analogy with the electron and muon, we might expect the magnetic moments to be

$$\hat{\boldsymbol{\mu}}_{\rm p} = \frac{e}{m_{\rm p}} \hat{\boldsymbol{S}}_{\rm p} \;; \qquad \hat{\boldsymbol{\mu}}_{\rm n} = 0 \qquad\qquad \left(\gamma_S = \frac{q}{m}\right)$$

-- These naïve expectations fail badly: introducing the *nuclear magneton* $\mu_{\rm N}$,

$$\boxed{\mu_{\rm N} \equiv \frac{e\hbar}{2m_{\rm p}} \approx 5.05 \times 10^{-27}\,{\rm J\,T^{-1}} \approx 3.15 \times 10^{-8}\,{\rm eV\,T^{-1}}}$$

and defining proton and neutron g-factors $g_{\rm p}$ and $g_{\rm n}$ such that (slide 3.32)

$$\hat{\boldsymbol{\mu}}_{\rm p} = g_{\rm p} \frac{\mu_{\rm N}}{\hbar} \hat{\boldsymbol{S}}_{\rm p} \;, \quad \mu_{\rm p} = \frac{g_{\rm p}}{2} \mu_{\rm N} \;; \qquad \hat{\boldsymbol{\mu}}_{\rm n} = g_{\rm n} \frac{\mu_{\rm N}}{\hbar} \hat{\boldsymbol{S}}_{\rm n} \;, \quad \mu_{\rm n} = \frac{g_{\rm n}}{2} \mu_{\rm N}$$

we naïvely expect $g_{\rm p} = 2$, $\mu_{\rm p} = \mu_{\rm N}$ and $g_{\rm n} = 0$, $\mu_{\rm n} = 0$, but instead find

G. Schneider et al., Science **358** (2017) 1081

$$\mu_{\rm p} = +2.79284734462(82)\,\mu_{\rm N} \;; \qquad g_{\rm p} \approx +5.586$$

$$\mu_{\rm n} = -1.91304273(45)\,\mu_{\rm N} \;; \qquad g_{\rm n} \approx -3.826$$

Magnetic moments : the proton

-- The magnetic moment of the proton was first measured (1933) by Stern :

$$\mu_{\rm p} = (2.5 \pm 10\%)\,\mu_{\rm N}$$

I. Estermann and O. Stern, Z. fur Physik **85** (1933) 17

Not at all an easy experiment -- the proton magnetic moment is small :

$$m_{\rm p} \gg m_{\rm e} \quad \Rightarrow \quad \mu_{\rm N} \ll \mu_{\rm B}\ ; \quad \mu_{\rm p} \ll \mu_{\rm e}$$

Stern was strongly discouraged by theorists, including Pauli, from doing the experiment, because the answer was "obviously" (Dirac) $\mu_p = \mu_N$:

"If you enjoy doing difficult experiments, you can do them, but it is a waste of time and effort because the result is already known"

John S. Rigden, "Hydrogen, the Essential Element", p110 (Harvard Books, 2003)

I. Estermann, Am. J. Phys. **43** (1975) 661

-- With the benefit of hindsight, this was the first evidence that the proton was not a pointlike particle, but possessed internal structure (*quarks*)

→ we will see later that the observed value of μ_p can be understood in terms of the magnetic moments of the proton's constituent quarks

Magnetic moments : nuclei

-- Atomic nuclei come in all possible spins : $S = 0,\ 1/2,\ 1,\ 3/2,\ 2,\ 5/2,\ \ldots$

To generalise the definition of μ (slide 3.33) to arbitrary spin S, in place of the "spin-up" state $|\uparrow\rangle$, we consider the spin state $|S,m_S\rangle$ with the maximal possible value ($m_S = S$) of m_S, and define

$$\mu \equiv \left\langle\, S, m_S = S \,\middle|\, (\hat{\mu}_S)_z \,\middle|\, S, m_S = S \,\right\rangle$$

-- With $\hat{\boldsymbol{\mu}}_S = \gamma_S \hat{\mathbf{S}}$, the (scalar) magnetic moment μ is therefore

$$\boxed{\mu = \gamma_S S\hbar} \qquad\qquad \hat{S}_z|S,S\rangle = S\hbar|S,S\rangle$$

The g-factor definitions on slide 3.32 naturally generalise to nuclei as

$$\boxed{\mu = g_S \mu_{\mathrm{N}} S}$$

-- The spin precession frequency for nuclei is then (see slide 3.35)

$$\boxed{\omega_{\mathrm{s}} = \gamma_S B = \frac{\mu B}{S\hbar} = \frac{g_S \mu_{\mathrm{N}} B}{\hbar}}$$

Magnetic moments : nuclei (2)

-- In *atomic* physics, for the proton and for nuclei, it is more usual to define the g-factors in terms of the Bohr magneton μ_B, rather than μ_N :

$$\hat{\boldsymbol{\mu}}_\mathrm{p} = -g_\mathrm{p}\frac{\mu_\mathrm{B}}{\hbar}\hat{\boldsymbol{S}}_p \; ; \qquad g_\mathrm{p} \approx -\frac{m_\mathrm{e}}{m_\mathrm{p}} \times (2.793) \approx -0.0031$$

(and to use a different sign convention!)

-- The spin of the nucleus is usually denoted as I (whereas in nuclear physics and particle physics the standard notation is J) :

$$\hat{H}_B = -\hat{\boldsymbol{\mu}}_I \cdot \mathbf{B} = -\gamma_I \hat{\boldsymbol{I}} \cdot \mathbf{B} \; ; \qquad \hat{\boldsymbol{\mu}}_I = -g_I \frac{\mu_\mathrm{B}}{\hbar}\hat{\boldsymbol{I}}$$

For a single-electron atom for example, in atomic-style notation, the overall magnetic dipole contribution to the Hamiltonian is written as

$$\hat{H}_B = \frac{\mu_\mathrm{B}}{\hbar}(\hat{\boldsymbol{L}} + g_\mathrm{e}\hat{\boldsymbol{S}} + g_I\hat{\boldsymbol{I}}) \cdot \mathbf{B}$$

Magnetic moments : nuclei (3)

-- The "atomic" (g_I) and "nuclear" (g_J) g-factors are related by

$$g_I = -\frac{m_\mathrm{e}}{m_\mathrm{p}} g_J \approx -\frac{1}{1836}\, g_J$$

$(\omega_\mathrm{s} = 2\pi\nu_\mathrm{s})$

particle	spin	"nuclear physics" $\mu = g_J \mu_\mathrm{N} J$		"atomic physics" $\mu = -g_I \mu_\mathrm{B} I$		spin precessn. frequency
	$J = I$	μ/μ_N	g_J	μ/μ_B	g_I	ν_s/B (MHz/T)
proton	$1/2$	$+2.793$	$+5.586$	$+0.00152$	-0.00304	42.6
neutron	$1/2$	-1.913	-3.826	-0.00104	$+0.00208$	29.2
^{4}He	0	0	0	0	0	0
^{6}Li	1	$+0.822$	$+0.822$	$+0.00045$	-0.00045	6.3
^{7}Li	$3/2$	$+3.256$	$+2.171$	$+0.00177$	-0.00118	16.5
^{85}Rb	$5/2$	$+1.353$	$+0.541$	$+0.00074$	-0.00029	4.1
^{87}Rb	$3/2$	$+2.750$	$+1.833$	$+0.00150$	-0.00100	14.0
^{107}Ag	$1/2$	-0.114	-0.228	-0.00006	$+0.00012$	1.7
^{109}Ag	$1/2$	-0.131	-0.262	-0.00007	$+0.00014$	2.0
e^-	$1/2$			-1.0011	$+2.0023$	28058.5
μ^-	$1/2$			-1.0011	$+2.0023$	135.5

The Stern-Gerlach Experiment

-- Classically, a magnetic dipole moment $\boldsymbol{\mu}$ in an external magnetic field $\mathbf{B}$ is subject to a couple

$$\mathbf{G} = \boldsymbol{\mu} \wedge \mathbf{B}$$

(leading to precession of $\boldsymbol{\mu}$ around $\mathbf{B}$, for example)

-- In addition, if the field $\mathbf{B}$ is *non-uniform*, then $\boldsymbol{\mu}$ is also subject to a force

$$\mathbf{F} = \boldsymbol{\nabla}(\boldsymbol{\mu} \cdot \mathbf{B})$$

For a sample of randomly oriented dipoles, the scalar product $\boldsymbol{\mu}\cdot\mathbf{B}$ takes on a continuous range of values between $-\mu B$ and $+\mu B$, leading, class-ically, to a continuum of possible trajectories through the magnetic field

-- In the *quantum* case, however, particles possessing an internal magnetic dipole moment $\boldsymbol{\mu}$ follow only a *finite number* of distinct spatial trajectories

This is a truly fundamental quantum effect, first demonstrated experimen-tally by Stern and Gerlach (1922)

Stern-Gerlach (2)

-- Consider a beam of *neutral* particles (e.g. neutrons) sent into a slowly varying magnetic field of the form

$$\mathbf{B}(\mathbf{r}) = \mathbf{B}_0 + \mathbf{B}_1(\mathbf{r})\,; \qquad |\mathbf{B}_1(\mathbf{r})| \ll |\mathbf{B}_0|$$

where $\mathbf{B}_0$ is constant, uniform and “large”, and $\mathbf{B}_1$ is “small” :

(S. Weinberg, “Lectures On Quantum Mechanics”, CUP, 2013, Chapter 4)

-- The field $\mathbf{B}_1$ must satisfy Maxwell’s equations,

$$\boldsymbol{\nabla} \cdot \mathbf{B}_1 = 0\ ; \qquad \boldsymbol{\nabla} \wedge \mathbf{B}_1 = 0$$

but its precise form is otherwise unimportant

-- Without loss of generality, orient the z axis along $\mathbf{B}_0$: $\mathbf{B}_0 = (0, 0, B_0)$

Let the particles have a magnetic dipole moment $\hat{\boldsymbol{\mu}}_S = \gamma_S \hat{\boldsymbol{S}}$

The motion of the particles through the magnetic field is then described by the Hamiltonian (from slide 3.27 with $q = 0$, and slide 3.34)

$$\boxed{\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \hat{\boldsymbol{\mu}}_S \cdot \mathbf{B} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \gamma_S\big(\hat{S}_z B_0 + \hat{\boldsymbol{S}} \cdot \mathbf{B}_1(\mathbf{r})\big)} \qquad \textbf{(3.64.1)}$$

Stern-Gerlach (3)

-- Expanded out, the Hamiltonian is

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} - \gamma_S\left(\hat{S}_z B_0 + \hat{S}_x B_{1,x}(\mathbf{r}) + \hat{S}_y B_{1,y}(\mathbf{r}) + \hat{S}_z B_{1,z}(\mathbf{r})\right)$$

-- Ehrenfest's theorem gives the equations of motion of the particle as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{r}}\rangle = \frac{i}{\hbar}\left\langle[\hat{H},\hat{\boldsymbol{r}}]\right\rangle \; ; \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{p}}\rangle = \frac{i}{\hbar}\left\langle[\hat{H},\hat{\boldsymbol{p}}]\right\rangle$$

-- The spin operator $\boldsymbol{S}$ commutes with the observables $\boldsymbol{r}$ and $\boldsymbol{p}$:

$$[\hat{\boldsymbol{S}},\hat{\boldsymbol{r}}] = 0 \; ; \qquad [\hat{\boldsymbol{S}},\hat{\boldsymbol{p}}] = 0$$

Hence, using the identity $\left[\hat{\boldsymbol{r}},\hat{\boldsymbol{p}}^2\right] = 2i\hbar\,\hat{\boldsymbol{p}}$ (see slide 1.14), we have

$$[\hat{H},\hat{\boldsymbol{r}}] = \frac{1}{2m}[\hat{\boldsymbol{p}}^2,\hat{\boldsymbol{r}}] = -\frac{i\hbar}{m}\hat{\boldsymbol{p}}$$

This gives (as expected on classical grounds)

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{r}}\rangle = \frac{1}{m}\langle\hat{\boldsymbol{p}}\rangle} \qquad \textbf{(3.65.1)}$$

Stern-Gerlach (4)

-- Similarly, we have

$$\left[\hat{H},\hat{\boldsymbol{p}}\right] = -\gamma_S\Big(\hat{S}_x\left[B_{1,x}(\mathbf{r}),\hat{\boldsymbol{p}}\right] + \hat{S}_y\left[B_{1,y}(\mathbf{r}),\hat{\boldsymbol{p}}\right] + \hat{S}_z\left[B_{1,z}(\mathbf{r}),\hat{\boldsymbol{p}}\right]\Big)$$

Applying the operator relation (slide 1.14 again)

$$\left[f(\mathbf{r}),\hat{\boldsymbol{p}}\right] = i\hbar(\boldsymbol{\nabla} f)$$

to each of the field components (B_x, B_y, B_z) gives

$$\left[\hat{H},\hat{\mathbf{p}}\right] = -i\hbar\gamma_S\Big(\hat{S}_x(\boldsymbol{\nabla} B_{1,x}(\mathbf{r})) + \hat{S}_y(\boldsymbol{\nabla} B_{1,y}(\mathbf{r})) + \hat{S}_z(\boldsymbol{\nabla} B_{1,z}(\mathbf{r}))\Big)$$

-- The second equation of motion is therefore

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{p}}\rangle &= \gamma_S\Big\langle\hat{S}_x(\boldsymbol{\nabla} B_{1,x}(\mathbf{r})) + \hat{S}_y(\boldsymbol{\nabla} B_{1,y}(\mathbf{r})) + \hat{S}_z(\boldsymbol{\nabla} B_{1,z}(\mathbf{r}))\Big\rangle \qquad \textbf{(3.66.1)}\\ &= \gamma_S\Big(\langle\hat{S}_x\rangle\langle\boldsymbol{\nabla} B_{1,x}(\mathbf{r})\rangle + \langle\hat{S}_y\rangle\langle\boldsymbol{\nabla} B_{1,y}(\mathbf{r})\rangle + \langle\hat{S}_z\rangle\langle\boldsymbol{\nabla} B_{1,z}(\mathbf{r})\rangle\Big)\end{aligned}$$

where, in the last step, each term has been factorised into its spin and spatial components

Stern-Gerlach (5)

-- Neglecting the contribution from the "small" field component $\mathbf{B}_1$ in equation (3.64.1), the spin component of the wavefunction evolves according to the Hamiltonian

$$\hat{H} = -\gamma_S \hat{S}_z B_0$$

i.e. to good approximation, the spin precesses about the "large" magnetic field $\mathbf{B}_0$, as in slides 3.34 - 3.40

-- Suppose the particle enters the Stern-Gerlach apparatus in the initial spin eigenstate $|sm_s\rangle$, as defined relative to the z axis (the direction of the "large" uniform field $\mathbf{B}_0$) :

$$|\psi(0)\rangle = |sm_s\rangle \ ; \qquad \hat{S}_z|sm_s\rangle = m_s\hbar|sm_s\rangle$$

Then, from equation (3.38.1), the expectation value $\langle \hat{\boldsymbol{S}} \rangle$ remains constant, and directed along z :

$$\langle\psi(t)|\hat{\boldsymbol{S}}|\psi(t)\rangle = (0, 0, m_s\hbar)$$

Stern-Gerlach (6)

-- In this case, only the z term of equation (3.66.1) is non-zero, giving the second equation of motion as

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\boldsymbol{p}}\rangle = \gamma_S \hbar m_s \langle \boldsymbol{\nabla} B_{1z}(\mathbf{r})\rangle}$$

-- Combining this with equation (3.65.1) then gives a second-order differential equation for the trajectory followed by the particle :

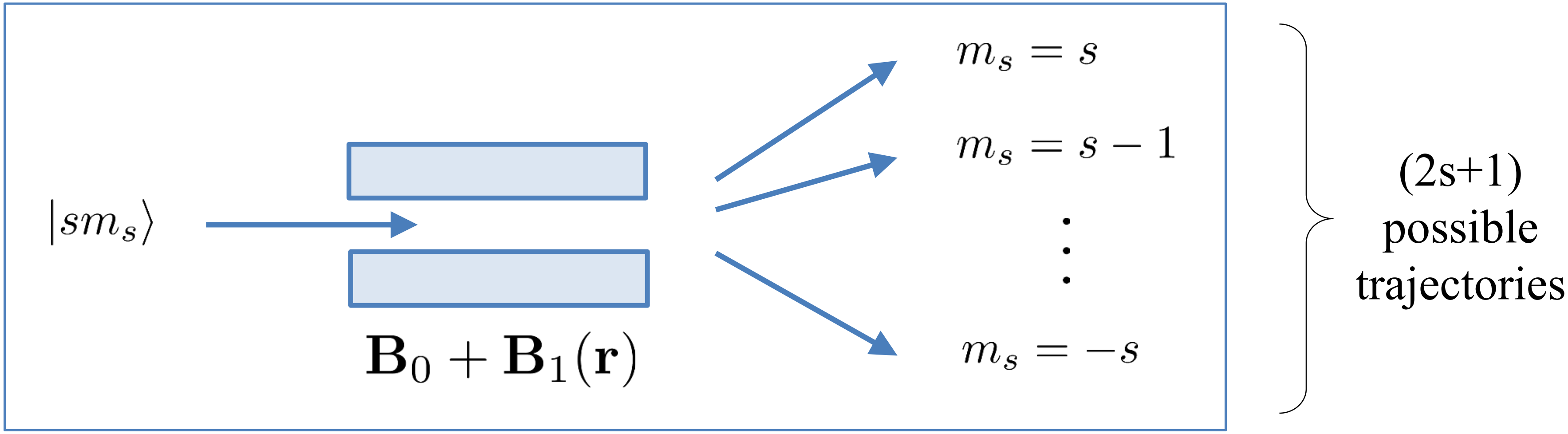
$$\boxed{m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{\boldsymbol{r}}\rangle = \gamma_S \hbar m_s \langle \boldsymbol{\nabla} B_{1z}(\mathbf{r})\rangle}$$

Each value of m_s gives rise to a different solution (trajectory) :

$$\langle\hat{\boldsymbol{r}}\rangle_{m_s}(t); \qquad (m_s = s, s-1, \ldots, -s)$$

Thus, whatever the form of $\mathbf{B}_1(\mathbf{r})$, there are $2s+1$ possible trajectories through the magnetic field, one for each possible value of m_s

Stern-Gerlach (7)



-- Note that, because we arbitrarily chose to orient the "large" magnetic field $\mathbf{B}_0$ along the z axis, it is the quantum number m_s defined with respect to z that has been picked out

(taking $\mathbf{B}_0$ along x would determine m_x, etc.)

-- The trajectories obtained are the same as would be obtained classically if the magnetic dipole moment could take on only the *quantised* values

$$\boldsymbol{\mu} = (0, 0, \gamma_S \hbar m_s)$$

Stern-Gerlach (8)

-- Now generalise to an arbitrary initial spin state

$$|\psi(0)\rangle = \sum_{m_s} c_{m_s} |s m_s\rangle$$

As on slides 3.39 - 3.40, we have precession at the Larmor frequency

$$\omega_\mathrm{s} = \gamma_S B_0$$

-- In practice, since B_0 is "large", the precession is extremely rapid on timescales associated with the motion through the magnetic field

Hence, when averaged over even short timescales, the x and y matrix elements *effectively* vanish :

$$\langle s m_s' | \hat{S}_x | s m_s \rangle = \langle s m_s' | \hat{S}_y | s m_s \rangle = 0$$

-- Only the z component is non-zero, as in equation (3.40.1) :

$$\boxed{\langle \psi(t) | \hat{S}_z | \psi(t) \rangle = \sum_{m_s} |c_{m_s}|^2 m_s \hbar}$$

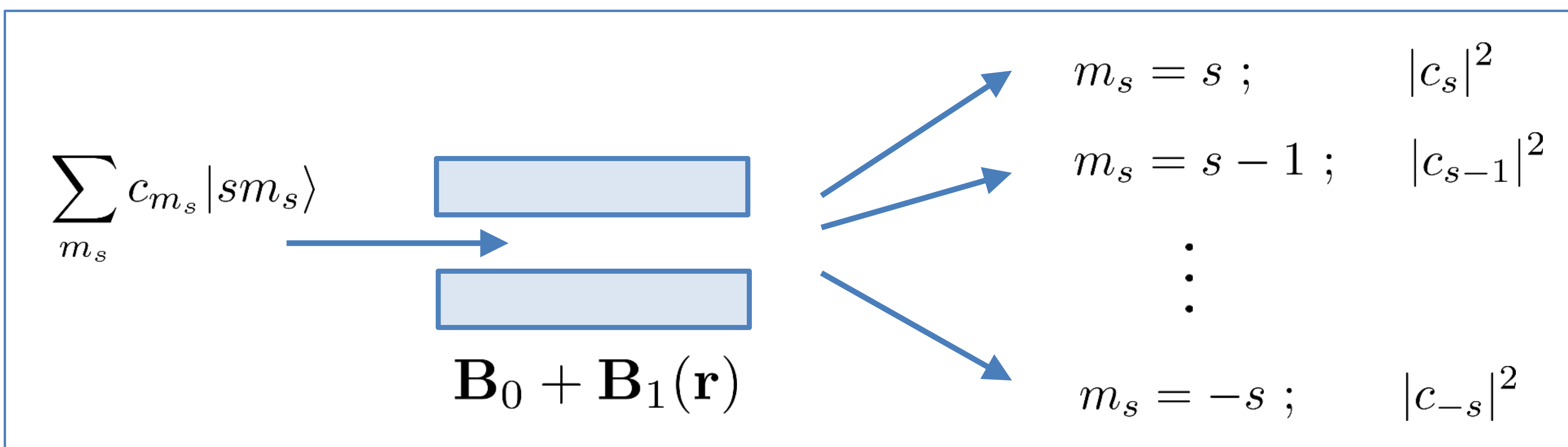
Stern-Gerlach (9)

-- Therefore, for a general initial spin state, the differential equation defining the average position of the particle is

$$\boxed{m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\hat{\mathbf{r}}\rangle = \gamma_S\hbar\sum_{m_s}|c_{m_s}|^2 m_s\langle\boldsymbol{\nabla}B_{1z}(\mathbf{r})\rangle} \qquad \textbf{(3.71.1)}$$

-- Thus a factor of $|c_{m_s}|^2$ is associated with each individual m_s trajectory

The incoming beam separates into $2s+1$ outgoing beams, each with different m_s, and with the intensity in each beam proportional to $|c_{m_s}|^2$:



Stern-Gerlach (10)

-- Note however that the analysis above has only determined how the *average position* of the particles in the original beam evolves with time

We have not actually shown that the original beam can *split* into two or more distinct outgoing beams, with well-defined spin states and intensities

[though equation (3.71.1) strongly suggests that this is what happens]

To demonstrate this fully requires a more involved analysis of the time evolution of the wavefunction, not just the average position

-- The S-G effect is of interest as a truly fundamental quantum phenomenon, but also finds many applications in the analysis or selection of spin states :

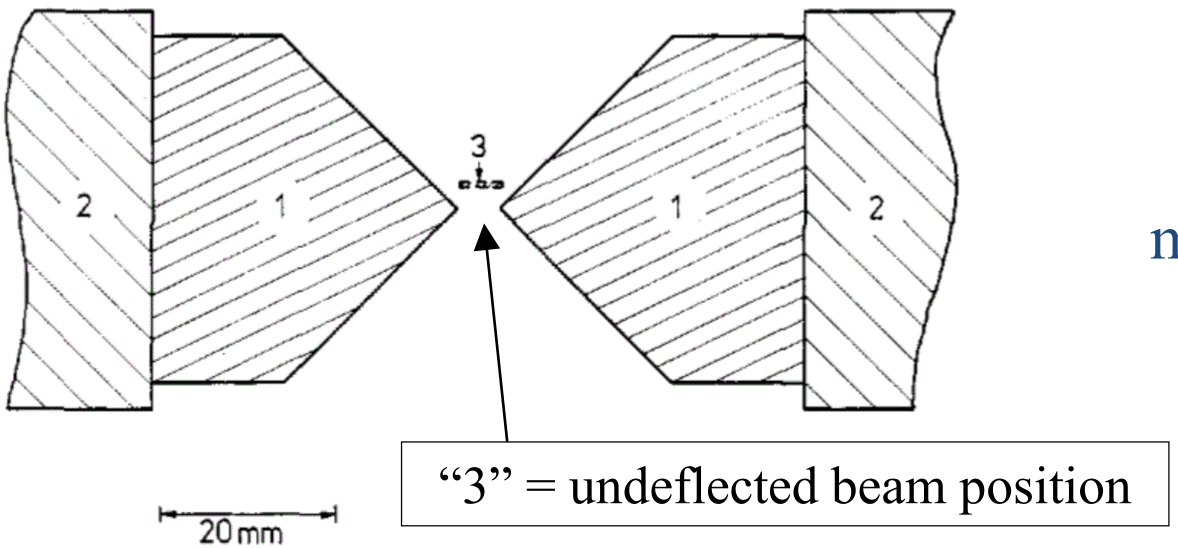
- observation of the trajectory followed by a particle tells us the value of the quantum number m_s
- particular spin states can be selected by blocking one or more of the emerging beams

Stern-Gerlach : a neutron polarimeter

-- As an example application, consider a Stern-Gerlach apparatus used to measure the polarisation of very low energy neutron beams :

T.J.L. Jones & W.G. Williams, J. Phys. E: Sci. Instrum. **13** (1980) 227

A non-uniform **B** field is produced using a dihedral magnet configuration :



max B ~ 2 T

max field gradient ~ 0.15 T/mm

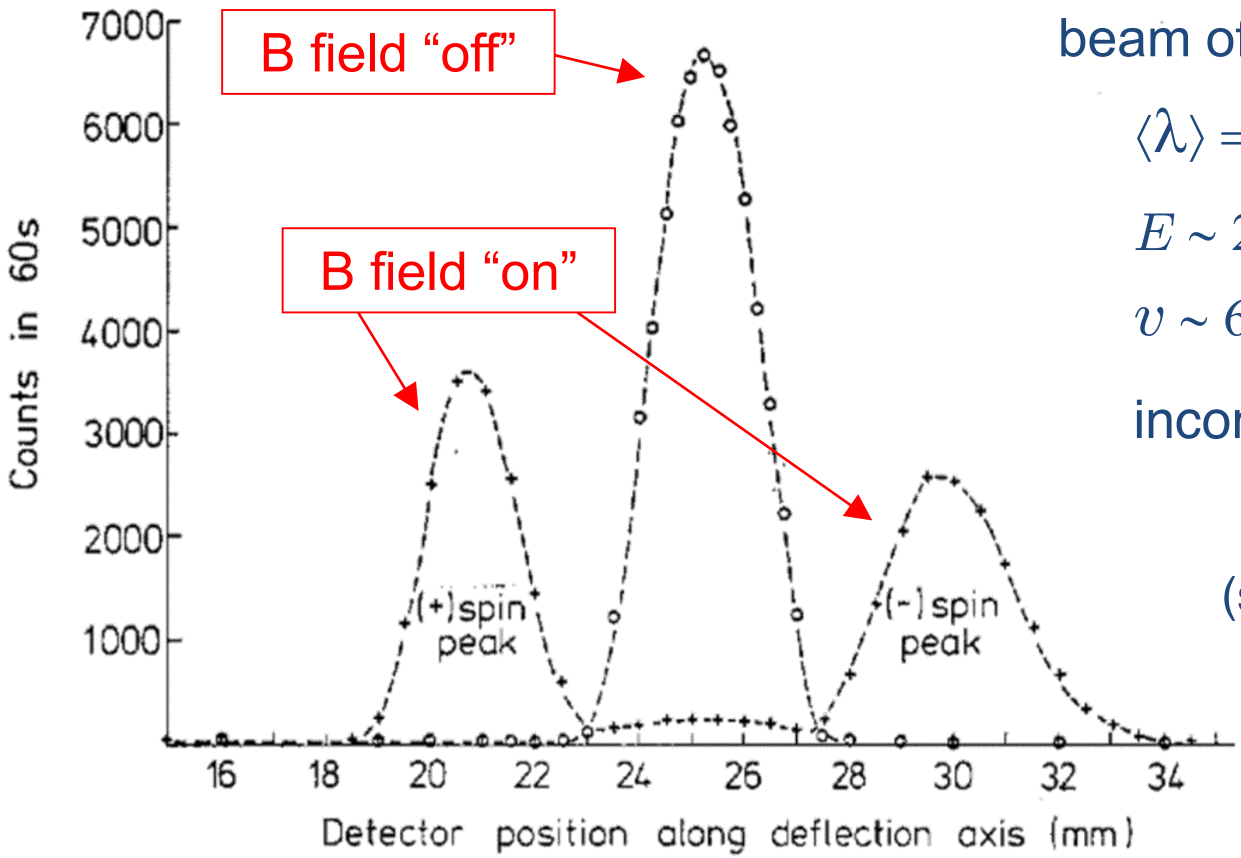
→

-- Neutrons were detected ~ 2.5 m beyond the magnet, giving a clear separation between the two emerging beams

(which have a finite width due to the spread of neutron velocities within the beam)

Stern-Gerlach : a neutron polarimeter

-- The relative area of the (+) and (–) peaks determines the polarisation of the incoming beam; the plot below is for *unpolarised* incoming neutrons :



beam of "cold" neutrons :

$$\langle \lambda \rangle = 0.67 \text{ nm}$$

$E \sim 2 \text{ meV}$ $T \sim 20 \text{ K}$

$v \sim 600 \text{ m s}^{-1}$

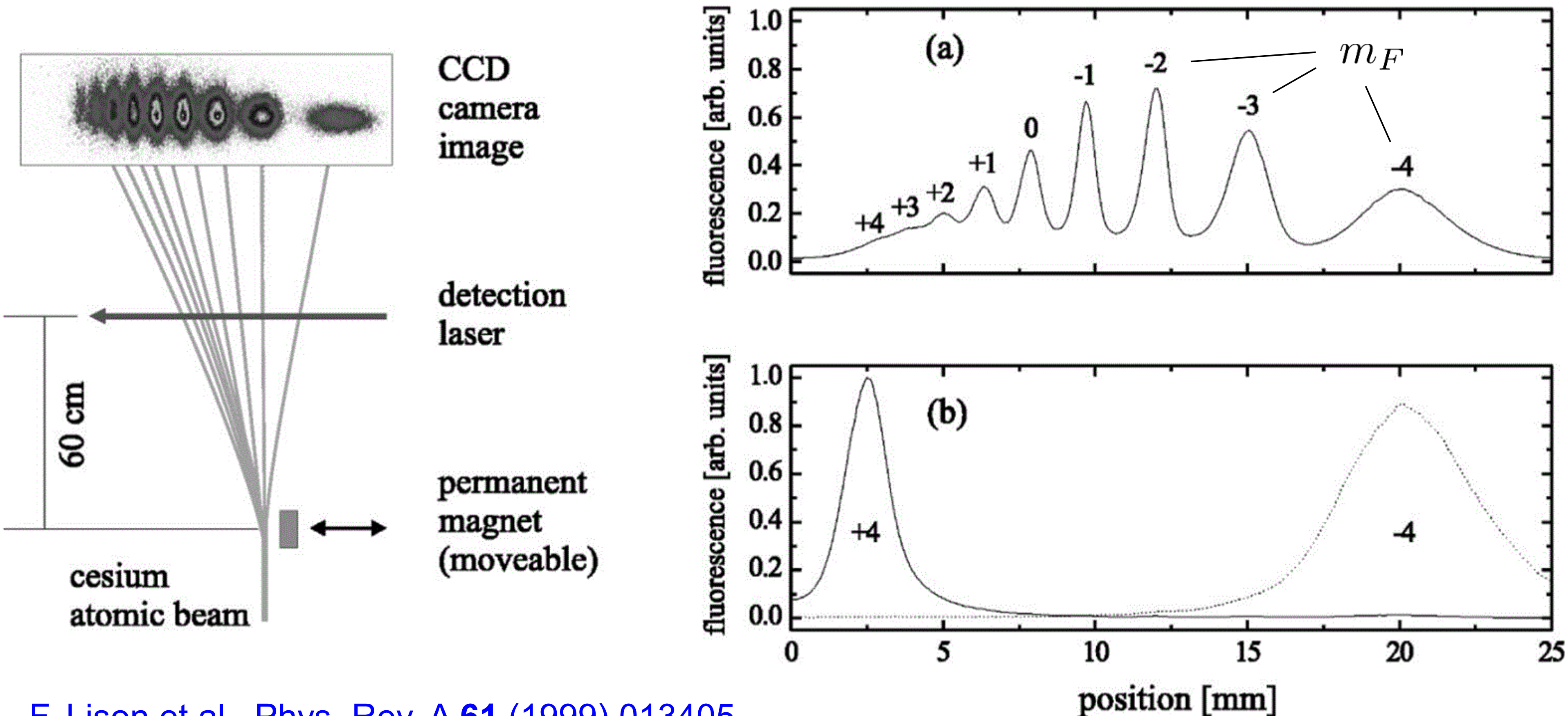
incoming flux $\sim 10^{10} \text{ m}^{-2} \text{ s}^{-1}$

(see 2 peaks : confirms that neutrons have spin 1/2 !)

-- The beam polarisation could be measured with 0.1% accuracy after about 1 hour of data collection

Stern-Gerlach : an atomic example

-- Another example, this time analysing a beam of (caesium) *atoms* :



F. Lison et al., Phys. Rev. A **61** (1999) 013405

-- The laser excites the atoms in the emerging beams; the resulting fluorescence is detected by a CCD camera, determining the beam positions

Stern-Gerlach : an atomic example (2)

-- The total internal angular momentum of an atom is

$$\hat{\boldsymbol{F}} = \hat{\boldsymbol{I}} + \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$$

$$\begin{cases} \hat{\boldsymbol{I}} = \text{nuclear spin} \\ \hat{\boldsymbol{L}} = \text{electron orbital a.m.} \\ \hat{\boldsymbol{S}} = \text{electron spin} \end{cases}$$

-- The caesium atom contains a nucleus ($Z = 55,\ A = 133$) of spin $I = 7/2$, and has a single valence electron ($S = 1/2$) with $L = 0$ in the ground state

Hence the caesium atom ground state is a mixture of states with total angular momentum $F = 3$ and $F = 4$:

$$F = I \otimes L \otimes S = \tfrac{7}{2} \otimes 0 \otimes \tfrac{1}{2} = 3, 4$$

-- The beam has been set up to contain only caesium atoms with $F = 4$:

- In the upper plot, the beam is a mixture of all possible m_F states

  → the atomic beam separates into $2F + 1 = 9$ beams, each corresponding to a different state $|F = 4\,, m_F\rangle$

- In the lower plot, the atoms have been *optically pumped* (see later) into one of the states $|F, m_F\rangle = |4,+4\rangle$ or $|4,-4\rangle$

  → only the $m_F = +4$ or $m_F = -4$ beam is seen

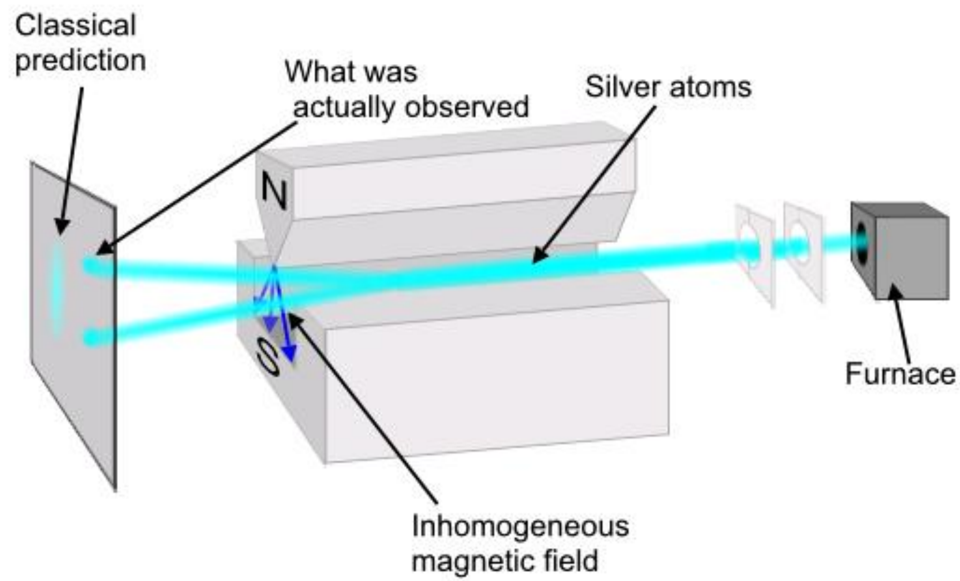
Stern-Gerlach : original observation

-- The original S-G experiment used a beam of neutral silver atoms :

W. Gerlach & O. Stern, Zeit. f. Physik **9** (1922) 349

Two distinct emerging beams were observed

At the time (1922), this was erroneously interpreted as confirmation of Bohr's postulate of "space quantisation"

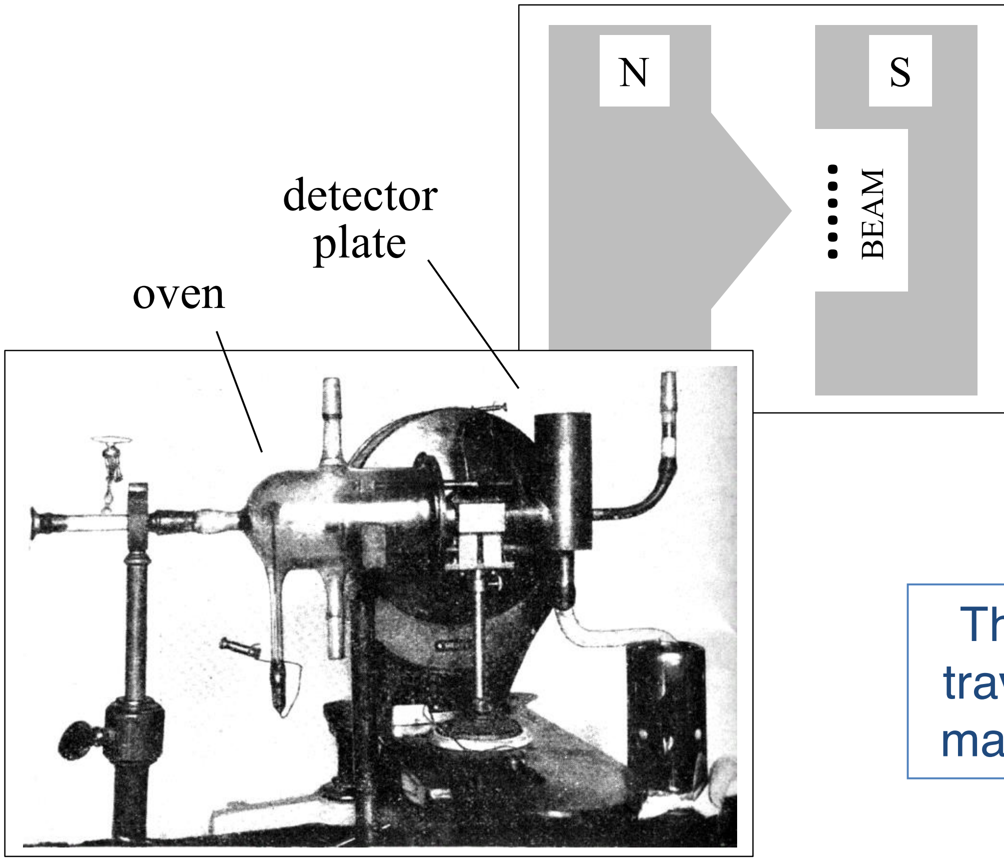


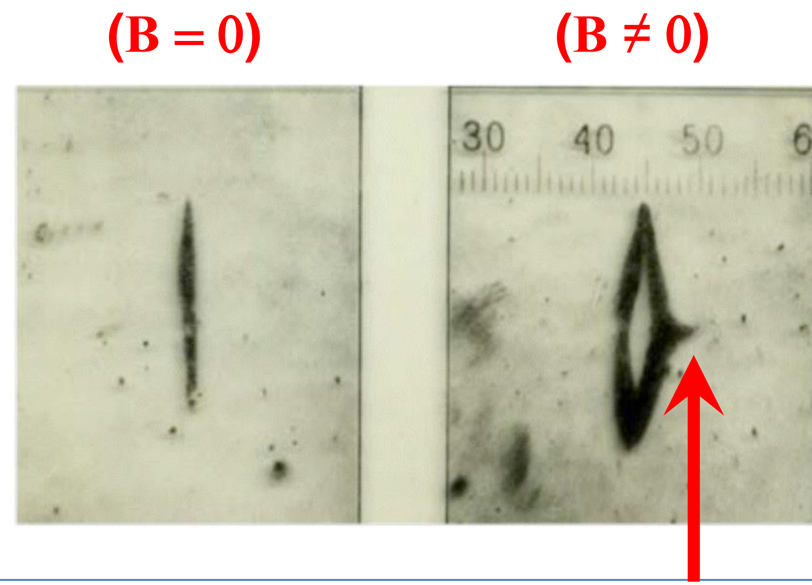
-- It was not until 1927 that the observation was correctly interpreted in terms of spin

[The suggestion that the electron might possess an internal angular momentum and an internal magnetic moment was first made by Goudsmit and Uhlenbeck in 1925, as an ad-hoc explanation of various features of atomic spectra and the Zeeman effect]

Stern-Gerlach : original observation (2)

-- Stern and Gerlach used a magnet with $B \sim 0.1$ T, $\nabla B \sim 10$ T/cm, acting over a distance ~ 3.5 cm, and obtained a beam separation of about 2 mm :





The “cusp” is due to beam particles which travel relatively close to the pointy bit of the magnet, where the field gradient is stronger

-- The experiment pioneered the use of atomic and molecular beams, and was far from easy …

J. Toennies et al., arXiv:1109.4864 (2011)

Stern-Gerlach : original observation (3)

Anyone who has not been through it cannot at all imagine how great were the difficulties with an oven to heat the silver up . . . within an apparatus which could not be fully heated [the seals would melt] and where a vacuum . . . had to be produced and maintained for several hours. The pumping speed . . . was ridiculously small compared with the performance of modern pumps. And . . . the pumps were made of glass and quite often they broke, either from the thrust of boiling mercury . . . or from the dripping of condensed water vapor. In that case the several-day effort of pumping, required during the warming up and heating of the oven, was lost. Also, one could be by no means certain that the oven would not burn through during the four- to eight-hour exposure time. Then both the pumping and the heating of the oven had to be started from scratch. It was a Sisyphus-like labor and the main load and responsibility was carried on the broad shoulders of Professor Gerlach. . . . He would get in about 9 p.m. equipped with a pile of reprints and books. During the night he then read the proofs and reviews, wrote papers, prepared lectures, drank plenty of cocoa or tea and smoked a lot. When I arrived the next day at the Institute, heard the intimately familiar noise of the running pumps, and found Gerlach still in the lab, it was a good sign: nothing broke during the night.[17]

W. Schütz, Phys. Blätter **25** (1969) 472

B. Friedrich and D. Herschbach, Daedalus **127** (1998) 165

Stern-Gerlach : original observation (4)

-- The fact that *two* emerging beams were observed suggests that silver atoms in their ground state have a total angular momentum $F = 1/2$

But this is *not* the case ...

-- Silver has a nucleus of spin $I = 1/2$, and a single valence electron with $L = 0$, $S = 1/2$, and so is a mixture of four states with $F = 0$ or $F = 1$:

$$F = I \otimes L \otimes S = \tfrac{1}{2} \otimes 0 \otimes \tfrac{1}{2} = 0, 1$$

$$|F, m_F\rangle = |1, +1\rangle,\ \ |1, 0\rangle,\ \ |1, -1\rangle,\ \ |0, 0\rangle$$

Hence we might expect to observe *three* emerging beams (not two), corresponding to the m_F values $m_F = -1, 0, +1$

-- Caesium and silver differ only in their nuclear spin I ; why then does caesium give $2F + 1 = 9$ beams, but silver *not* give $2F + 1 = 3$ beams ?

$\rightarrow$ the explanation needs an understanding of *hyperfine structure* and the *Zeeman effect* (see later)

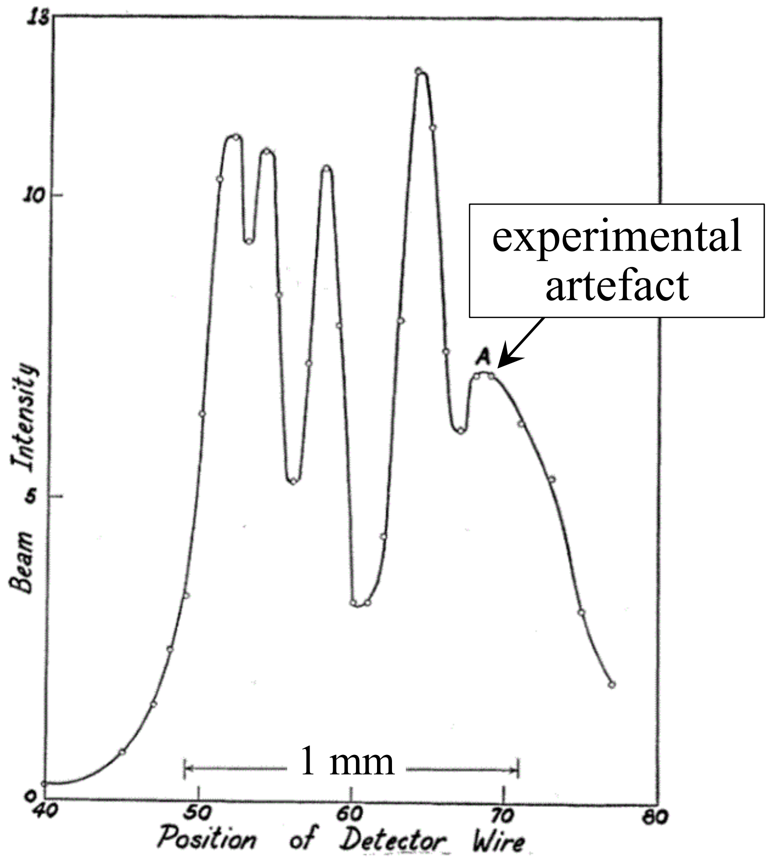
Stern-Gerlach : measurement of nuclear spin

-- As a final example, in the early 1930's, using atomic beams, Isidor Rabi demonstrated that a succession of *three* S-G apparatuses

(one with "large" $\mathbf{B}$, one with "small" $\mathbf{B}$, one with *reversed* "large" $\mathbf{B}$)

could be configured to measure *nuclear spins* :

-- e.g. using a beam of neutral sodium atoms :



Four peaks were observed, establishing directly that $2I+1=4$;

$\rightarrow$ the sodium nucleus has spin $I=3/2$

I. I. Rabi & V. W. Cohen, Phys. Rev. **43** (1933) 582

Stern-Gerlach : measurement of nuclear spin (2)

-- The thoughts of Victor Cohen, in the early hours of the morning, going home on the NY subway and surveying his fellow passengers :

> "I know something that none of you know; I am the only person in the world who knows that the nuclear spin of sodium is 3/2"

John S. Rigden, "Rabi, Scientist and Citizen", Chapter 5 (Basic Books Inc., 1987)

-- By the end of the 1930's, with the addition of alternating electric fields to drive transitions between spin states, this work had led to the development of the *molecular beam resonance* method :

→ *Rabi oscillations*

→ precise measurements of nuclear magnetic moments

(more on this later) and eventually

→ NMR spectroscopy, MRI scanners, masers, atomic clocks, …

Landau Levels

-- Classically, a particle undergoing circular orbits in a magnetic field B can have a continuous range of energies, depending on the orbital radius r :

$$E = \frac{1}{2} m r^2 \omega_\mathrm{c}^2 \ ; \qquad \omega_\mathrm{c} = \frac{|q| B}{m}$$

-- In the *quantum* case however, the orbital energies can become quantised into discrete *Landau levels* :

→ highly degenerate states, with a uniform energy spacing proportional to the applied magnetic field B

-- Quantum effects (Landau levels) are usually irrelevant, but can become important especially for large magnetic fields and low temperatures

This leads to various interesting effects in condensed matter physics ;

→ we will consider in particular the *Quantum Hall Effect* …

Landau Levels (2)

-- From slide 3.4, the appropriate Hamiltonian operator (in any gauge, and neglecting spin) is

$$\boxed{\hat{H} = \frac{1}{2m}\left[\hat{\boldsymbol{p}} - q\mathbf{A}(\mathbf{r},t)\right]^2 = \frac{1}{2m}\hat{\mathbf{\Pi}}^2} \qquad \textbf{(3.84.1)}$$

where the vector operator $\mathbf{\Pi}$ is defined as

$$\hat{\mathbf{\Pi}} \equiv \hat{\boldsymbol{p}} - q\mathbf{A}(\mathbf{r},t) \; ; \qquad \hat{\mathbf{\Pi}}^2 = \hat{\Pi}_x^2 + \hat{\Pi}_y^2 + \hat{\Pi}_z^2$$

-- The components of $\mathbf{\Pi}$ do not commute; for example

$$\left[\hat{\Pi}_x, \hat{\Pi}_y\right] = \left[\hat{p}_x - qA_x, \hat{p}_y - qA_y\right] = -q\left[A_x, \hat{p}_y\right] - q\left[\hat{p}_x, A_y\right]$$

Using the identities (slide 1.14)

$$\left[A_x, \hat{p}_y\right] = i\hbar\frac{\partial A_x}{\partial y} \; , \qquad \left[A_y, \hat{p}_x\right] = i\hbar\frac{\partial A_y}{\partial x}$$

then gives

$$\left[\hat{\Pi}_x, \hat{\Pi}_y\right] = -iq\hbar\left(\frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial x}\right) = iq\hbar(\mathbf{\nabla}\wedge\mathbf{A})_z = iq\hbar\, B_z$$

Landau Levels (3)

-- Introduce non-Hermitian operators a and $a^\dagger$ defined as

$$\hat{a} = \sqrt{\frac{1}{2q\hbar B}}\left(\hat{\Pi}_x + i\hat{\Pi}_y\right) \;\; ; \qquad \hat{a}^\dagger = \sqrt{\frac{1}{2q\hbar B}}\left(\hat{\Pi}_x - i\hat{\Pi}_y\right)$$

The commutator of the operators a and $a^\dagger$ is

$$[\hat{a}, \hat{a}^\dagger] = -\frac{i}{q\hbar B}[\hat{\Pi}_x, \hat{\Pi}_y] = \frac{B_z}{B}$$

For a uniform magnetic field $\mathbf{B} = (0,0,B_z)$, we therefore have

$$[\hat{a}, \hat{a}^\dagger] = 1$$

-- The operator product $a^\dagger a$ is

$$\begin{aligned}
\hat{a}^\dagger \hat{a} &= \frac{1}{2q\hbar B}(\hat{\Pi}_x - i\hat{\Pi}_y)(\hat{\Pi}_x + i\hat{\Pi}_y) \\
&= \frac{1}{2q\hbar B}(\hat{\Pi}_x^2 + \hat{\Pi}_y^2 + i[\hat{\Pi}_x, \hat{\Pi}_y]) \\
&= \frac{1}{2q\hbar B}(\hat{\mathbf{\Pi}}^2 - \hat{\Pi}_z^2) - \frac{1}{2}
\end{aligned}$$

Landau Levels (4)

-- Hence the Hamiltonian $H = \mathbf{\Pi}^2/2m$ of equation (3.84.1) can be written as

$$\boxed{\hat{H} = \hbar\omega_{\mathrm{c}}\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right) + \frac{1}{2m}\hat{\Pi}_z^2} \qquad \omega_{\mathrm{c}} \equiv \frac{|q|B}{m}$$

where ω_{c} is the cyclotron frequency of slide 3.36

-- The first term in the Hamiltonian above corresponds to a quantum harmonic oscillator with energy eigenvalues

$$E_{\nu} = \hbar\omega_{\mathrm{c}}\left(\nu_{\mathrm{L}} + \frac{1}{2}\right) \quad ; \qquad \nu_{\mathrm{L}} = 0, 1, 2, \ldots$$

Hence the Π_x and Π_y terms in the Hamiltonian H, transverse to the magnetic field $\mathbf{B}$, contribute quantised *Landau levels* with energy spacing

$$\boxed{\Delta E = \hbar\omega_{\mathrm{c}} = \frac{\hbar|q|B}{m}} \qquad \textbf{(3.86.1)}$$

Landau Levels (5)

-- For example : for an electron in a magnetic field $B = 1\ \mathrm{T}$, the separation between neighbouring Landau levels is

$$\Delta E = \hbar\omega_{\mathrm{c}} = \frac{\hbar e B}{m_{\mathrm{e}}} \approx 1.2 \times 10^{-4}\,\mathrm{eV}$$

-- At room temperature, this is swamped by thermal effects :

$$T = 300\,\mathrm{K} \;\Rightarrow\; k_{\mathrm{B}}T \approx 2.6 \times 10^{-2}\,\mathrm{eV} \ll \Delta E$$

→ large magnetic fields and low temperatures are needed for quantum effects (Landau levels) to become significant

e.g. $T = 1.5\,\mathrm{K} \;\Rightarrow\; k_{\mathrm{B}}T \approx 1.3 \times 10^{-4}\,\mathrm{eV} \sim \Delta E$

The Landau gauge

-- The analysis so far has been gauge independent, but we can also choose to work in a particular gauge; a type of Coulomb gauge known as the *Landau gauge* is especially convenient :

$$\boxed{\mathbf{A}(\mathbf{r}) = (-By, 0, 0)}$$

$$\mathbf{B} = \boldsymbol{\nabla} \wedge \mathbf{A} = (0, 0, B)$$

$$\boldsymbol{\nabla} \cdot \mathbf{A} = 0$$

-- In the Landau gauge, the Hamiltonian becomes

$$\hat{H} = \frac{1}{2m_{\mathrm{e}}} \left[(\hat{p}_x - eBy)^2 + \hat{p}_y^2 + \hat{p}_z^2 \right]$$

-- The Schrödinger equation $\hat{H}\psi = E\psi$ now admits separated variable solutions of the form

$$\psi(\mathbf{r}) = e^{i(k_x x + k_z z)} \chi(y)$$

[EXAMPLES SHEET]

where k_x and k_z are constants, and $\chi(y)$ is a solution of the equation

$$\hat{H}_\chi \chi(y) \equiv \frac{1}{2m_{\mathrm{e}}} \left[(\hbar k_x - eBy)^2 + \hat{p}_y^2 + \hbar^2 k_z^2 \right] \chi(y) = E\chi(y)$$

The Landau gauge (2)

-- The Hamiltonian H_χ has the form of a simple harmonic oscillator :

$$\hat{H}_\chi = \frac{\hat{p}_y^2}{2m_\mathrm{e}} + \frac{1}{2}m\omega_c^2(y-y_0)^2 + \frac{\hbar^2 k_z^2}{2m_\mathrm{e}}$$

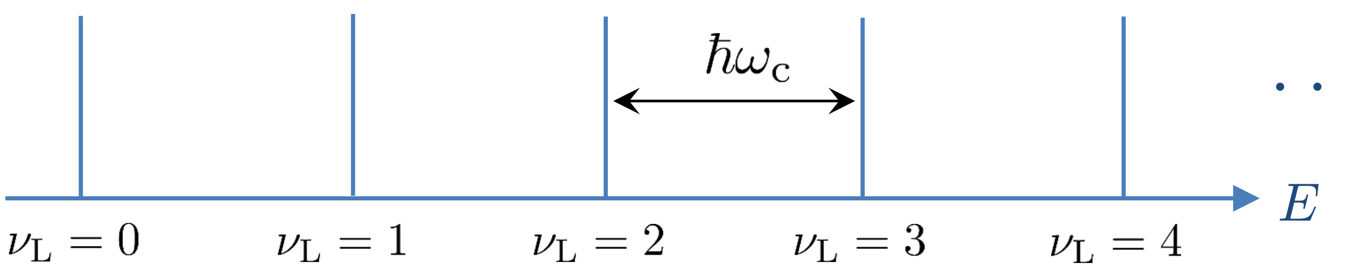
The angular frequency of the harmonic oscillator is $\omega = \omega_\mathrm{c}$ (the cyclotron frequency), and its central position is $y = y_0$, where

$$y_0 = \frac{\hbar k_x}{eB} \qquad \textbf{(3.89.1)}$$

-- The energy eigenvalues are

$$\boxed{E_{\nu,k_z} = \left(\nu_\mathrm{L} + \frac{1}{2}\right)\hbar\omega_\mathrm{c} + \frac{\hbar^2 k_z^2}{2m_\mathrm{e}}} \qquad (\nu_\mathrm{L} = 0, 1, 2, \ldots)$$

This corresponds to a set of Landau levels for each possible value of k_z :



The Landau gauge (3)

-- To take the spin of the electron into account, an extra term should be included in the Hamiltonian :

$$-(\hat{\boldsymbol{\mu}}_S)_{\mathrm{e}} \cdot \mathbf{B} = \left(\frac{e}{2m_{\mathrm{e}}} g_{\mathrm{e}} \hat{\mathbf{S}} \right) \cdot \mathbf{B} = \frac{eB}{2m_{\mathrm{e}}} g_{\mathrm{e}} \hat{S}_z = \frac{\omega_{\mathrm{c}}}{2} g_{\mathrm{e}} \hat{S}_z$$

-- For a “spin-up” electron, this gives an extra contribution

$$\Delta E = g_e \frac{\omega_{\mathrm{c}}}{2} \langle \uparrow | \hat{S}_z | \uparrow \rangle = \frac{g_e}{2} \frac{\hbar \omega_{\mathrm{c}}}{2} \; ,$$

and similarly for “spin-down”, with opposite sign; thus, including spin, the energy eigenvalues become

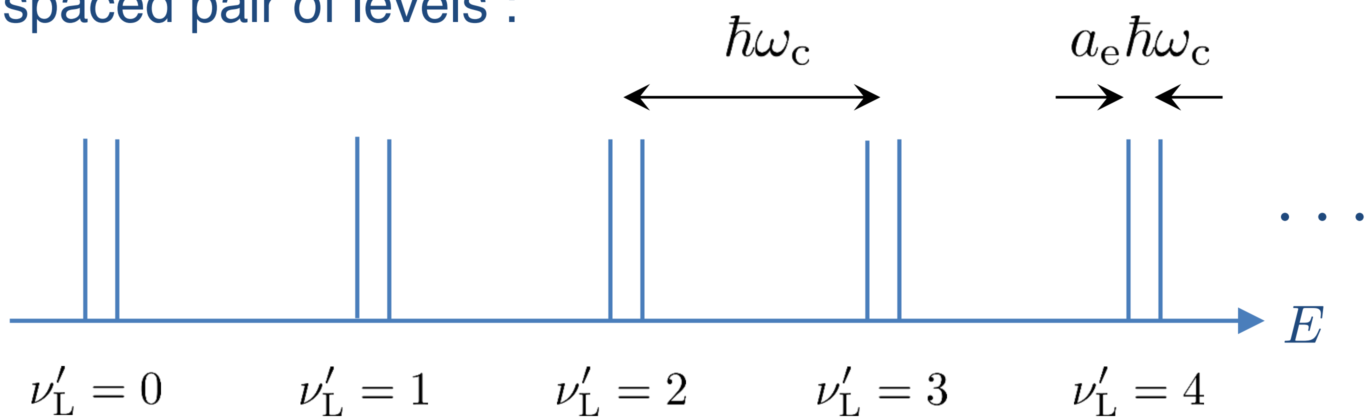
$$\boxed{E_{\nu, k_z} = \left(\nu_{\mathrm{L}} + \frac{1}{2} \pm \frac{1}{2} \frac{g_{\mathrm{e}}}{2} \right) \hbar \omega_{\mathrm{c}} + \frac{\hbar^2 k_z^2}{2m_{\mathrm{e}}}}$$

-- In the approximation $g_{\mathrm{e}} = 2$, this again gives Landau levels with uniform energy separation $\hbar\omega_{\mathrm{c}}$ (but with a different energy offset) :

$$E_{\nu, k_z} = \nu'_{\mathrm{L}} \hbar \omega_{\mathrm{c}} + \frac{\hbar^2 k_z^2}{2m_{\mathrm{e}}} \qquad (\nu'_{\mathrm{L}} = 0, 1, 2, \ldots)$$

The Landau gauge (4)

-- For the more precise value $g_e \cong 2.0023$, each Landau level splits into a closely spaced pair of levels :



where a_e is the *anomalous magnetic moment* of the electron,

$$a_e \equiv \frac{g_e - 2}{2} \approx 0.0012$$

-- The effects of Landau levels are typically observed in systems where electrons are confined to a boundary layer between two different materials

$\rightarrow$ *two-dimensional electron systems* (2DES)

The z contribution can then be neglected; we effectively have $k_z = 0$

The 2D Electron Gas (2DEG)

-- Consider a layer of electrons confined to the plane $z = 0$ within a two-dimensional region of area $A = L_x \times L_y$:

$$-\frac{L_x}{2} < x < \frac{L_x}{2} \; ; \qquad -\frac{L_y}{2} < y < \frac{L_y}{2}$$

-- Consider first the case with no magnetic field ($\mathbf{B} = 0$) :

The density of available states per unit area, $g(E)$, for a 2D gas of particles is independent of energy (see Appendix B) :

$$g(E) = \frac{1}{A}\frac{\mathrm{d}N}{\mathrm{d}E} = \frac{m_{\mathrm{e}}}{\pi\hbar^2} \qquad \textbf{(3.92.1)}$$

where a factor of two has been included to account for the electron spin

-- For a system containing a total of N electrons, all available states are occupied up to a maximum energy E_{F}, the *Fermi energy*, given by

$$N = g(E)AE_{\mathrm{F}} = \frac{m_{\mathrm{e}}A}{\pi\hbar^2}E_{\mathrm{F}} \qquad \textbf{(3.92.2)}$$

The 2D electron gas (2)

-- Now apply a uniform magnetic field $\mathbf{B} = (0,0,B)$ along z :

In the approximation $g_{\mathrm{e}} = 2$, we obtain Landau levels with constant energy spacing

$$\Delta E = \hbar\omega_{\mathrm{c}} = \frac{\hbar e B}{m_{\mathrm{e}}} \qquad \textbf{(3.93.1)}$$

-- In the Landau gauge $\mathbf{A} = (-By,0,0)$, the eigenstates in a given Landau level have the form

$$\psi(\mathbf{r}) = e^{ik_x x}\chi(y)$$

Assuming that the spread of the harmonic oscillator wavefunctions $\chi(y)$ along y is much less than L_y , then the central position y_0 of each oscillator is restricted to the range

$$|y_0| < \frac{L_y}{2}$$

-- From equation (3.89.1), this in turn restricts the possible values of k_x :

$$\left|\frac{\hbar k_x}{eB}\right| < \frac{L_y}{2} \quad \Rightarrow \quad |k_x| < \frac{eBL_y}{2\hbar}$$

The 2D electron gas (3)

-- Hence the number of available states N_L in each Landau level is

$$N_\mathrm{L} = \frac{2|k_x|_\mathrm{max}}{(\pi/L_x)} = \frac{eBL_y}{\hbar(\pi/L_x)} = \frac{eBA}{\pi\hbar} = \frac{2eBA}{h} = \frac{2\Phi}{\Phi_0} \qquad \textbf{(3.94.1)}$$

where $\Phi_0 \equiv h/e \approx 4.1 \times 10^{-15}\ \mathrm{T.m}^2$ (the *flux quantum* again)

The number of states per unit area, n, in each Landau level is then

$$\boxed{n \equiv \frac{N_\mathrm{L}}{A} = \frac{2B}{\Phi_0}} \qquad \textbf{(3.94.2)}$$

-- Each Landau level is *highly degenerate* :

e.g. for $B = 5\ \mathrm{T}$, and a 2D electron gas confined to an area $A = 1\ \mathrm{mm}^2$, the number of available states in each level is

$$N_\mathrm{L} = \frac{2BA}{\Phi_0} \approx \frac{2 \times 5 \times (10^{-3})^2}{(4 \times 10^{-15})} = 2.5 \times 10^9$$

-- As a cross-check of equation (3.94.2), we can verify that the total number of available states in a field B is the same as for zero-field …

The 2D electron gas (4)

-- With *no* magnetic field, the density of available states $g(E)$ is independent of energy, and given by equation (3.92.1)

For an energy interval equal to the Landau level spacing $\Delta E = \hbar\omega_{\mathrm{c}}$ of equation (3.93.1), the number of states per unit area at *zero field* is then

$$n = g(E)\Delta E = g(E)\hbar\omega_{\mathrm{c}} = \frac{m_{\mathrm{e}}}{\pi\hbar^2}\frac{\hbar eB}{m_{\mathrm{e}}} = \frac{2eB}{h} = \frac{2B}{\Phi_0}$$

This is equation (3.94.2) again; i.e. the total number of states is preserved

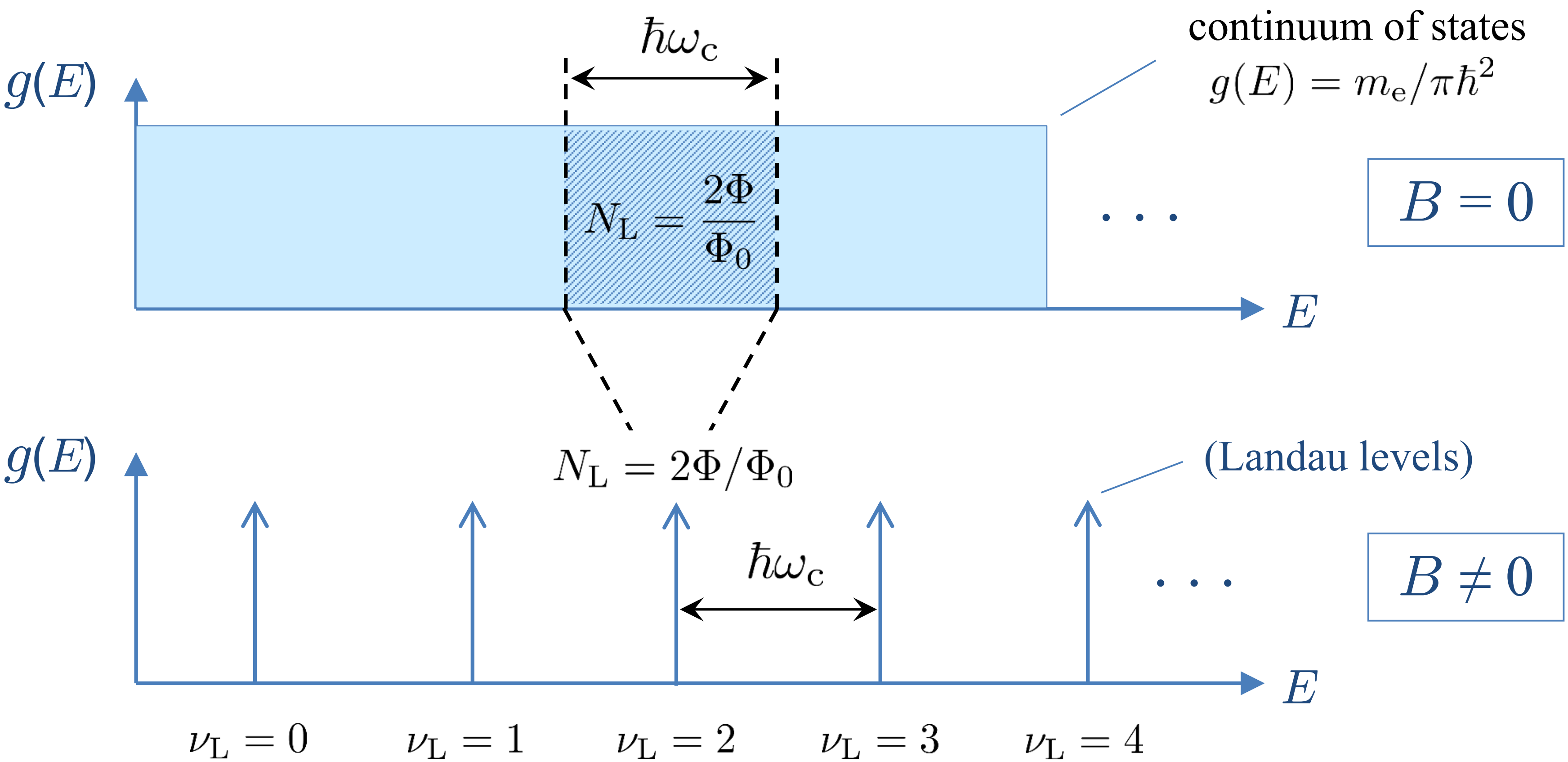
-- Thus, when the magnetic field B is applied :

→ the density of states $g(E)$ changes from a constant, uniform distribution in energy to a set of discrete, highly degenerate Landau levels, separated in energy by $\Delta E = \hbar\omega_{\mathrm{c}}$

→ the number of states in each Landau level is the same as the number of zero-field states contained in an energy interval $\Delta E = \hbar\omega_{\mathrm{c}}$

The 2D electron gas (5)

-- In summary, the effect of "switching on" the magnetic field is to transform the zero-field, uniform density of states $g(E)$ …



… into a set of equally spaced δ-functions, while preserving the total number of available states

The 2D electron gas (6)

-- For a total of N electrons, since there are $N_\mathrm{L} = nA$ available states per level, the number of fully occupied Landau levels is

$$n_\mathrm{L} = \mathrm{int}\left[\frac{N}{N_\mathrm{L}}\right]$$

A fraction

$$f_\mathrm{L} = \frac{N}{N_\mathrm{L}} - n_\mathrm{L} = \frac{N}{N_\mathrm{L}} - \mathrm{int}\left[\frac{N}{N_\mathrm{L}}\right] \qquad (0 \leq f_\mathrm{L} \leq 1)$$

of the highest non-empty Landau level is occupied

-- Using equations (3.92.2) and (3.94.1), the ratio N/N_L above is

$$\frac{N}{N_\mathrm{L}} = \frac{m_\mathrm{e} A}{\pi \hbar^2} E_\mathrm{F} \times \frac{\pi\hbar}{eBA} = \frac{E_\mathrm{F}}{\hbar\omega_c} \; ; \qquad \omega_c \equiv \frac{eB}{m_\mathrm{e}}$$

The fraction f_L can thus be expressed in terms of the Fermi energy, E_F, as

$$\boxed{f_\mathrm{L} = \frac{E_\mathrm{F}}{\hbar\omega_\mathrm{c}} - \mathrm{int}\left[\frac{E_\mathrm{F}}{\hbar\omega_\mathrm{c}}\right]}$$

The 2D electron gas (7)

-- Thus, as B increases, f_{L} is periodic with a period given by

$$\Delta\left(\frac{E_{\mathrm{F}}}{\hbar\omega_{\mathrm{c}}}\right) = 1 \qquad \Rightarrow \qquad \frac{E_{\mathrm{F}} m_{\mathrm{e}}}{\hbar e}\Delta\left(\frac{1}{B}\right) = 1$$

-- Hence many properties of a metal show a periodicity in $1/B$, with a period

$$\boxed{\Delta\left(\frac{1}{B}\right) = \frac{\hbar e}{m_{\mathrm{e}} E_F}}$$

electrical resistivity $\rightarrow$ the *Shubnikov-de Haas effect*

magnetic susceptibility $\rightarrow$ the *de Haas-van Alphen effect*

(see next term's Part II Quantum Condensed Matter Physics course)

-- However, by far the most striking and unexpected manifestation of Landau levels in 2D electron gases is the *Quantum Hall Effect* (*QHE*) …

(also covered in next term's QCMP course)

The Quantum Hall Effect

NON-EXAMINABLE

-- The *Hall effect* is the generation of a transverse potential difference across a conductor carrying current when it is placed in a magnetic field

First observed by Edwin Hall in 1879 E. Hall, Am. J. Math. **2** (1879) 287

This *classical* Hall effect (CHE) arises from the transverse Lorentz force on the current-carrying electrons, and has many modern applications (e.g. Hall probes to measure magnetic field strengths, …)

-- In 1980, at high field and low temperature, von Klitzing, Dorda and Pepper unexpectedly observed dissipationless current flow with remarkably constant and reproducible Hall resistivities : the *quantum* Hall effect (QHE)

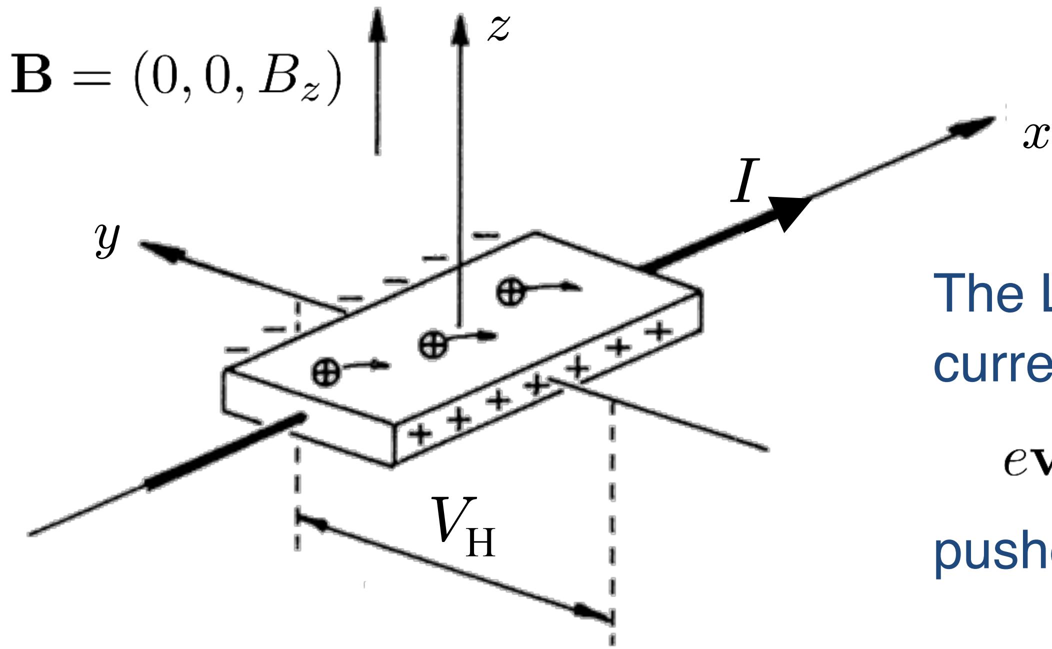
K. v.Klitzing, G. Dorda & M. Pepper, Phys. Rev. Lett. **45** (1980) 494

-- Before discussing the QHE, we need to review the CHE …

This is all ***non-examinable***

The classical Hall effect

-- Consider a two-dimensional conductor in a perpendicular magnetic field :



The Lorentz force on conventional current carriers (charge $+e$)

$$e\mathbf{v} \wedge \mathbf{B} = e(v_y B_z, -v_x B_z, 0)$$

pushes them in the $-y$ direction

-- Adding the magnetic field $\mathbf{B}$ therefore leads to a transverse potential difference, known as the *Hall voltage*, V_{H}

-- Experimentally : apply a known V and B, and measure V_{H} and I

(V is the longitudinal potential, along x)

The classical Hall effect (2)

-- For a homogenous, isotropic substance, the current densities (currents per unit length) J_x, J_y and the electric field components E_x, E_y are related as

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix} \qquad \begin{cases} \rho_{yy} = \rho_{xx} \\ \rho_{yx} = -\rho_{xy} \end{cases}$$

-- If we allow only *longitudinal* current flow (i.e. $J_y = 0$), then the longitudinal and transverse resistivities are given by

$$\rho_{xx} = \frac{E_x}{J_x} \; ; \qquad \rho_{xy} = -\frac{E_y}{J_x}$$

-- In the Drude model of electrical conduction, the electrons undergo multiple, random, elastic scatters with the impurities in the sample, leading to a constant electron drift velocity $\mathbf{v}$ such that

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{e}{m^*}\mathbf{E} - \frac{e}{m^*}(\mathbf{v} \wedge \mathbf{B}) - \frac{\mathbf{v}}{\tau}$$

where τ is the mean time between collisions

The classical Hall effect (3)

-- Under steady state conditions ($\partial v/\partial t = 0$), this becomes

$$v_x = -\frac{\omega_c^* \tau}{B} E_x - \omega_c^* \tau v_y \; ; \qquad v_y = -\frac{\omega_c^* \tau}{B} E_y + \omega_c^* \tau v_x$$

where

$$\omega_c^* \equiv \frac{eB}{m^*}$$

Since no current is allowed to flow in the y direction ($v_y = 0$), we have

$$v_x = \frac{E_y}{B} \qquad \textbf{(3.102.1)}$$

-- The longitudinal current density J_x is (by definition)

$$J_x = -e n_e v_x \qquad \textbf{(3.102.2)}$$

where n_e is the electron number density (# per unit area)

Eliminating v_x between equations (3.102.1) and (3.102.2) then gives

$$\rho_{xy} = -\frac{E_y}{J_x} = \frac{B}{n_e e}$$

The classical Hall effect (4)

-- If the sample has width w, and carries current I, then

$$J_x = \frac{I}{w}\,; \qquad E_y = -\frac{V_\mathrm{H}}{w} \qquad \Rightarrow \qquad \rho_{xy} = -\frac{E_y}{J_x} = \frac{V_\mathrm{H}}{I}$$

Hence the (transverse) *Hall resistivity* can be obtained from the measur-able quantities V_H and I as

$$\boxed{\rho_{xy} = \frac{V_\mathrm{H}}{I} = \frac{B}{n_\mathrm{e} e}} \qquad \textbf{(3.103.1)}$$

Classically, we therefore expect the Hall resistivity ρ_{xy} to be proportional to the applied field B; the measured slope allows the electron density n_e to be determined

-- If the sample has length L, then the (longitudinal) Ohmic resistance is

$$\frac{V}{I} = \frac{E_x L}{J_x w} = \frac{L}{w}\frac{E_x}{J_x} = \frac{L}{w}\rho_{xx} \qquad \Rightarrow \qquad \boxed{\rho_{xx} = \frac{w}{L}\frac{V}{I}}$$

This allows the longitudinal resistivity, ρ_{xx} , to be obtained from the meas-urable quantities V and I , and the known dimensions of the sample

The (Integer) Quantum Hall Effect

-- Experimentally, at low temperature :

- At low magnetic field, the expected linear increase of ρ_{xy} with B is observed, equation (3.103.1), from which n_{e} can be determined

- But, at high magnetic field, unexpectedly,

dissipationless flow ($\rho_{xx} = 0$) is observed over extended ranges of B within which ρ_{xy} is remarkably constant

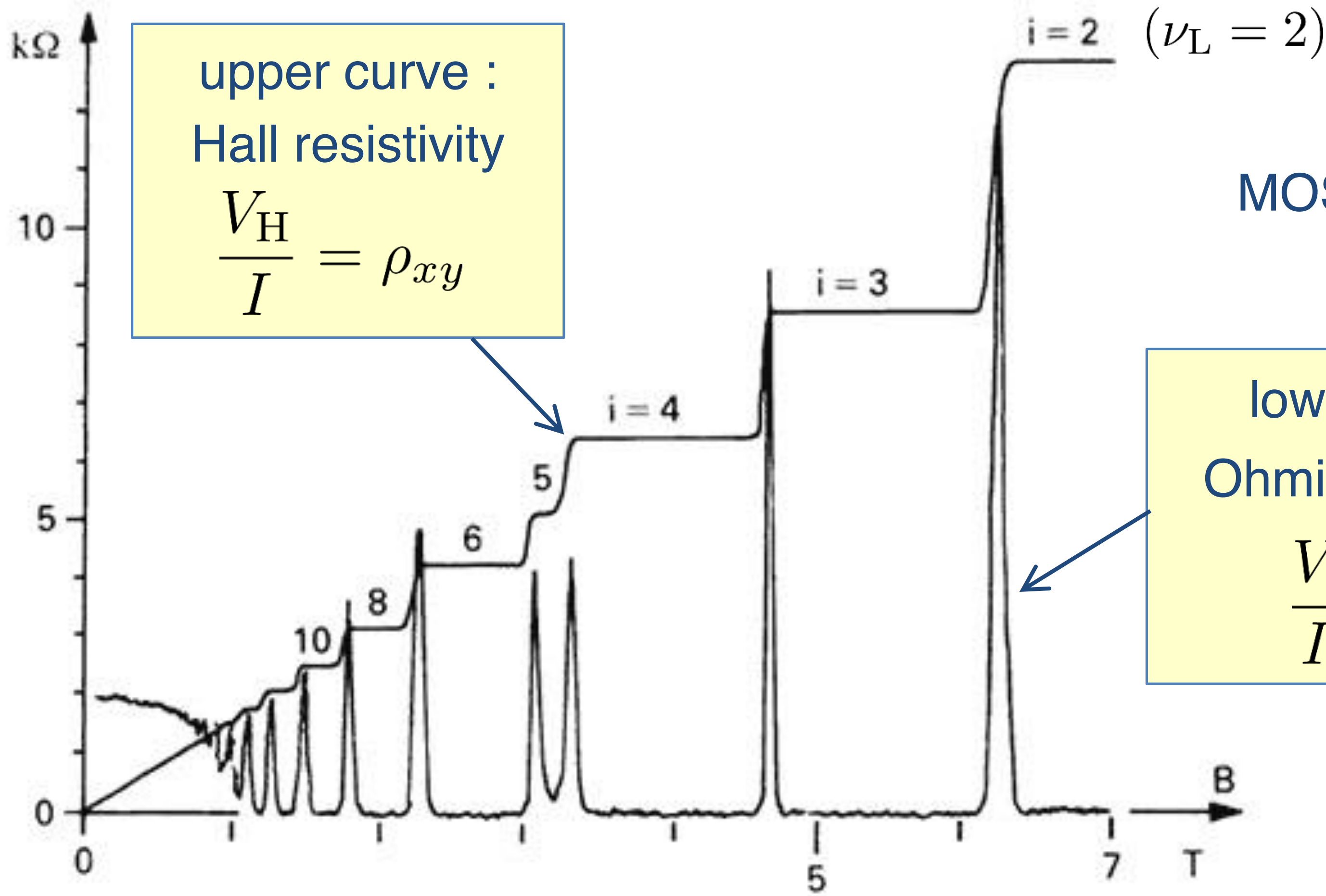
$\rightarrow$ the (*integer*) *Quantum Hall Effect* (IQHE)

K. v.Klitzing, G. Dorda & M. Pepper, Phys. Rev. Lett. **45** (1980) 494

-- The original discovery was made in MOSFET devices ("metal-oxide-semiconductor field-effect transistor")

The QHE has since been studied in a wide variety of materials, especially in GaAs/AlGaAs heterostructures, and in silicon

The Quantum Hall Effect (2)



MOSFET, $T = 1.5$ K

The plateau regions are observed to have to Hall resistivity values given by

$$\rho_{xy} = \frac{1}{\nu_L}\frac{h}{e^2} \approx \frac{1}{\nu_L}\frac{6.626\times 10^{-34}}{(1.6\times 10^{-19})^2} \approx \frac{25.88}{\nu_L}\,\mathrm{k}\Omega$$

The Quantum Hall Effect (3)

-- In each *plateau region* ($\nu_L = 1,2,3,\ldots$) , the transverse resistivity values

$$\rho_{xy} = \frac{R_\mathrm{K}}{\nu_\mathrm{L}} \; ; \qquad R_\mathrm{K} \equiv \frac{h}{e^2}$$

are found to be reproducible to high precision across different samples and materials (to better than 3 parts in 10^9)

-- The transverse resistivities seen in the plateau regions can equivalently be expressed as

$$\sigma_{xy} = \frac{1}{\rho_{xy}} = \nu_\mathrm{L} \frac{e^2}{h}$$

i.e. the transverse conductance is found to be quantised in units of e^2/h

-- The QHE has recently been seen also in graphene ;

(the electrons involved are *relativistic*; the QHE is similar in principle but the details differ) :

→ the value of R_K derived from graphene agrees with that from GaAs to better than 1 part in 10^{10}

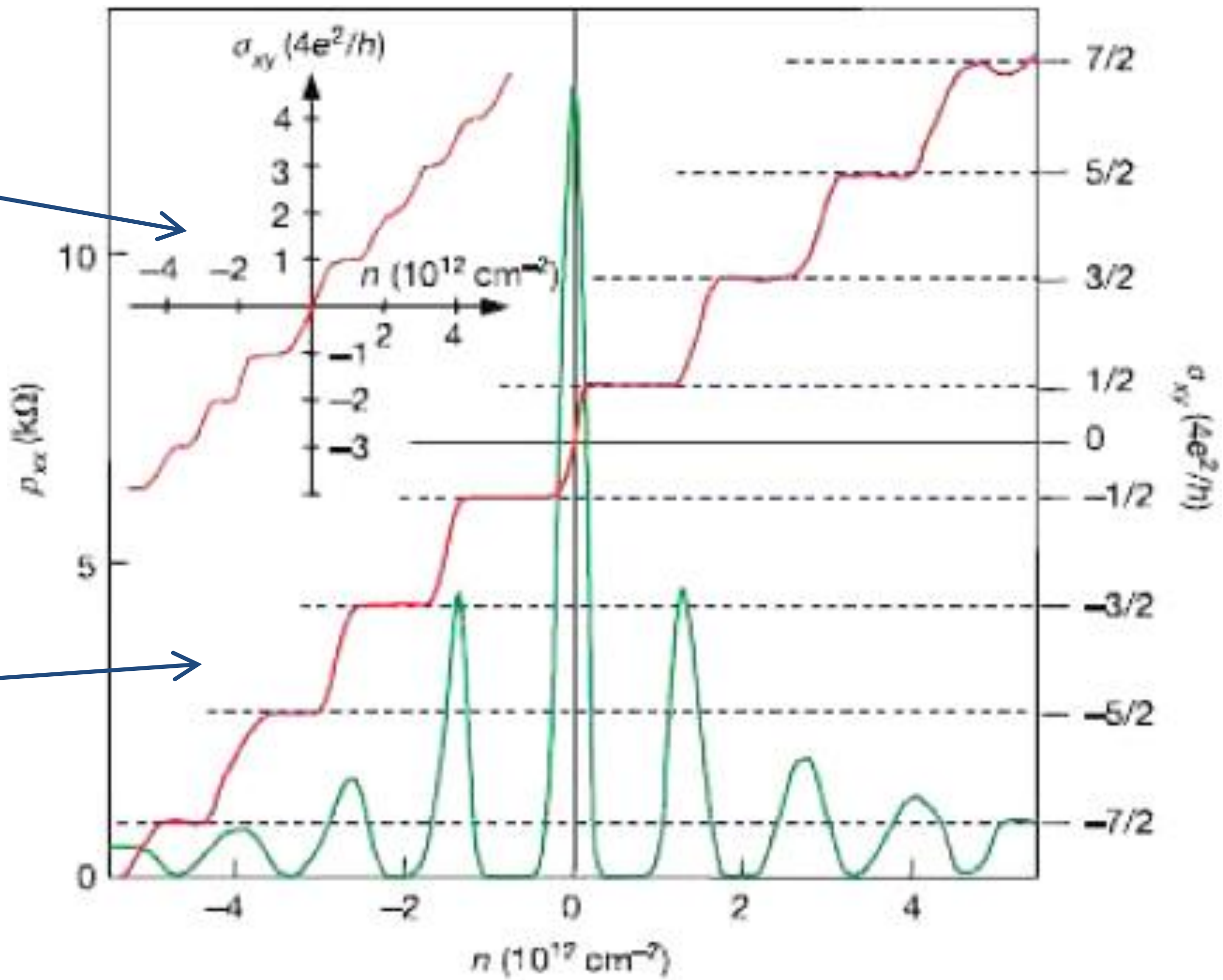
T. J. B. M. Janssen et al., Metrologia **49** (2012) 294

The Quantum Hall Effect (4)

-- Example of the Quantum Hall Effect in graphene :

double layer
(integer)

single layer
(half-integer)



K. S. Novoselov et al., Nature **438** (2005) 197

The Quantum Hall Effect (5)

How can these observations (the IQHE) be understood ?

-- At low temperature and high magnetic field, we expect quantum effects to become important :

$\rightarrow$ the cyclotron orbits become *quantised* (Landau levels)

-- Suppose we choose B such that the electrons exactly fill all of the available states in the first n_L Landau levels

(taking into account the splitting of each level into two for $g = 2.0023$)

From equation (3.94.2), the overall electron density (# per unit area) is then

$$n_{\mathrm{e}} = n_{\mathrm{L}} \frac{B}{\Phi_0} = n_{\mathrm{L}} \frac{eB}{h} \qquad (n_{\mathrm{L}} = 1, 2, 3, \ldots)$$

-- Since all available states in the highest occupied Landau level are filled, elastic scattering of electrons becomes impossible

(since the next accessible Landau level is $\hbar\omega_{\mathrm{c}}$ away)

$\Rightarrow$ at low enough temperatures, scattering becomes "frozen out"

The Quantum Hall Effect (6)

-- Hence, at special, critical values of the magnetic field corresponding to filled Landau levels,

$$B = \frac{1}{n_{\mathrm{L}}} \frac{n_{\mathrm{e}} h}{e}$$

we expect to see dissipationless current flow :

$$\rho_{xx} \to 0$$

-- From equation (3.103.1), the Hall resistivity ρ_{xy} for these values of B is

$$\boxed{\rho_{xy} = \frac{B}{n_e e} = \frac{1}{n_{\mathrm{L}}} \frac{h}{e^2}} \qquad \textbf{(3.109.1)}$$

These values of ρ_{xy} , corresponding to full Landau levels, are precisely those observed in the IQHE in the plateau regions

-- Full Landau levels are clearly involved in the QHE, *but* …

The Quantum Hall Effect (7)

-- The analysis so far leaves two critical questions unanswered :

(1) Why is dissipationless flow observed over *extended ranges* of B (plateau regions), not just at certain critical values of B ?

(with rapid jumps to the next plateau)

(2) Why are the observed plateau resistivities found to be the same to such high precision across different samples and materials ?

-- The answers are complex, and are an interplay of the following ingredients:

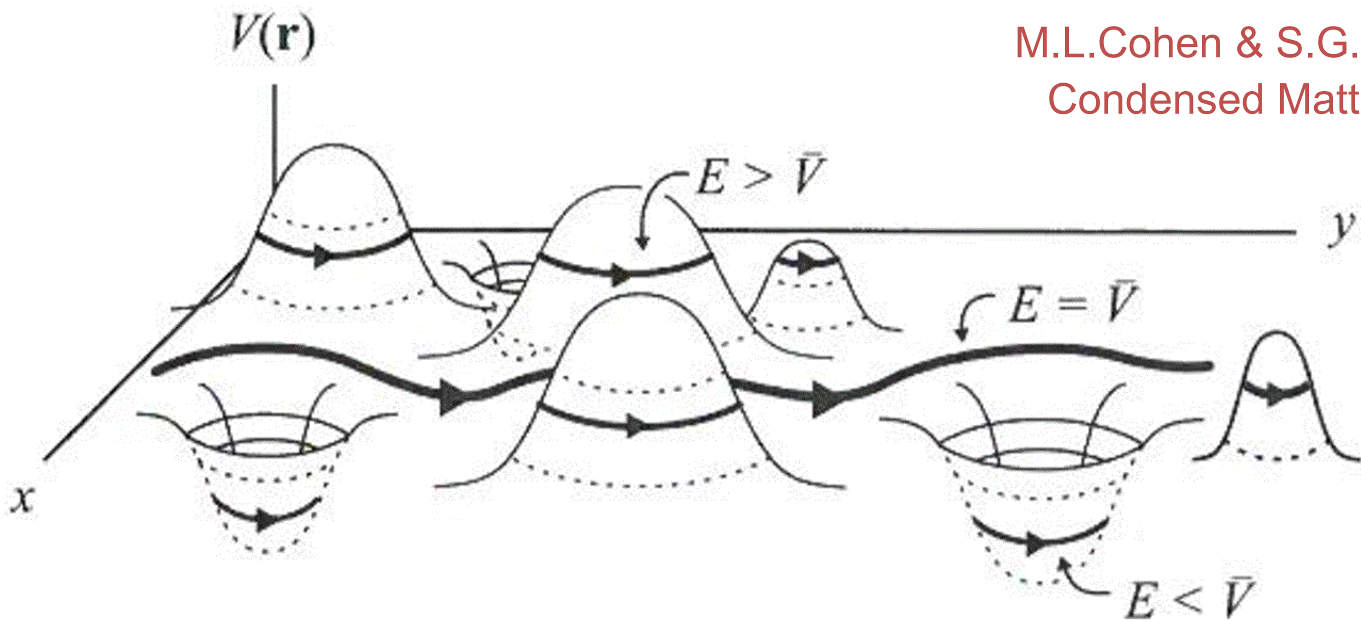
- the (inevitable) presence of *disorder* in the material;
- the consequences of *gauge invariance* ;
- the existence of *edge states* in Quantum Hall systems;

A woefully vague and incomplete account of these effects now follows …

(see for example www.damtp.cam.ac.uk/user/tong/qhe.html for the gory details)

The Quantum Hall Effect (8)

-- The appearance of plateau regions with dissipationless flow relies on the (inevitable) presence of *disorder* in the material :



M.L.Cohen & S.G.Louie, "Fundamentals of Condensed Matter Physics", CUP (2016)

-- The disorder spreads out the well-defined Landau energies and introduces *localised states* at peaks and troughs in the bumpy potential

These localised states cannot contribute to conductivity (only extended states still with the Landau energies can do that)

→ the conductivity (resistivity) does not change as B is varied

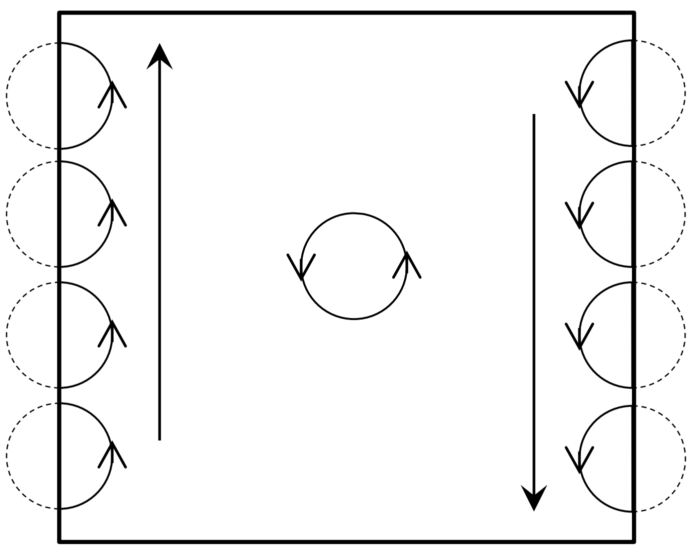
The Quantum Hall Effect (9)

-- Arguments based on gauge invariance then guarantee that the plateau values of the resistivity still take on the Landau level quantised values, equation (3.109.1), *even in the presence of disorder and impurities*

> "There's a wonderful irony in this; the glorious precision with which these integers ν are measured is due to the dirty, crappy physics of impurities."

D. Tong, arXiv:1606.06687 (2016), p48

-- The existence of edge states in Quantum Hall systems is also crucial :



Electrons "skip" along the edges, in one direction only

In Quantum Hall systems, gapless edge states lead to current flow without energy loss

(even in the presence of disorder)

The Quantum Hall Effect (10)

-- There are in fact three varieties of Quantum Hall Effect : "integer", "spin" and "anomalous", all of which have now been observed

see, for example : S. Oh, Science **340** (2013) 153

There are also "fractional" variants, where the integers n_{L} are replaced by rational numbers : 1/3, 1/5, 2/5, …

-- There are deep connections with *topology* ; study of the QHE has led to the field of *topological materials*

(the integers n_{L} are topological invariants known as *Chern numbers*)

-- The observation of these various new phases of condensed matter is of fundamental interest, and may also lead to novel devices and applications

e.g. new devices in data storage, data transfer, quantum computing

e.g. "spintronics" (= "spin electronics" = "spin transport electronics")

Appendices

-- *Appendix A :*

Derivation of the classical Hamiltonian for a charged particle moving in a given electromagnetic field

$$H = \frac{1}{2m}\left[\mathbf{p} - q\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t)$$

(covered in this term's Part II Optics & Electrodynamics course)

-- *Appendix B :*

The density of available states $g(E)$ for a free particle in 2D and in 3D

(covered in the Part IB Condensed Matter course, and elsewhere)

A : Classical Electrodynamics

-- In the Hamiltonian formulation of classical dynamics, the equations of motion of a particle with position and momentum coordinates

$$\mathbf{r} = (x_1, x_2, x_3) \; ; \qquad \mathbf{p} = (p_1, p_2, p_3)$$

are obtained from the classical Hamiltonian $H(x_j,p_j)$ via Hamilton's equations :

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = \frac{\partial H}{\partial p_j} \; ; \qquad \frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial H}{\partial x_j} \qquad (j = 1, 2, 3)$$

-- For example, for a non-relativistic particle moving in a potential $V(\mathbf{r})$, the Hamiltonian is

$$H = T + V = \frac{\sum_j p_j^2}{2m} + V(x_j)$$

Hamilton's equations give Newton's 2nd law of motion :

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = \frac{p_j}{m} \; ; \qquad \frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial V}{\partial x_j}$$

$$(\mathbf{p} = m\mathbf{v}) \qquad (\mathbf{F} = m\mathbf{a})$$

A : Classical Electrodynamics (2)

-- Motion in an electromagnetic field described by potentials $\mathbf{A}$ and ϕ is introduced via the "minimal substitution" prescription :

$$\boxed{\mathbf{p} \to \mathbf{p} - q\mathbf{A} \; ; \qquad E \to E + q\phi}$$

-- Applying minimal substitution to the free-particle Hamiltonian $H = \mathbf{p}^2/2m$ gives the classical Hamiltonian

$$\boxed{H = \frac{1}{2m}\left[\mathbf{p} - q\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t)}$$

-- To justify this form for H, we can check that the correct equation of motion (the Lorentz force equation) is obtained from Hamilton's equations …

-- To this end, write the Hamiltonian H as

$$H = \frac{\sum_k (p_k - qA_k)^2}{2m} + q\phi$$

-- The first Hamilton equation gives

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = \frac{\partial H}{\partial p_j} = \frac{1}{m}(p_j - qA_j) \tag{3.117.1}$$

-- The second Hamilton equation gives

$$\frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial H}{\partial x_j} = \frac{q}{m}\left[\sum_k (p_k - qA_k)\frac{\partial A_k}{\partial x_j}\right] - q\frac{\partial \phi}{\partial x_j}$$

$$= q\left[\sum_k \frac{\mathrm{d}x_k}{\mathrm{d}t}\frac{\partial A_k}{\partial x_j} - \frac{\partial \phi}{\partial x_j}\right]$$

A : Classical Electrodynamics (4)

-- Differentiating equation (3.117.1) with respect to t gives

$$m\frac{\mathrm{d}^2 x_j}{\mathrm{d}t^2} = \frac{\mathrm{d}p_j}{\mathrm{d}t} - q\frac{\mathrm{d}A_j}{\mathrm{d}t}$$

$$= q\left[\sum_k \frac{\mathrm{d}x_k}{\mathrm{d}t}\frac{\partial A_k}{\partial x_j} - \frac{\partial \phi}{\partial x_j}\right] - q\overbrace{\left[\frac{\partial A_j}{\partial t} + \sum_k \frac{\partial A_j}{\partial x_k}\frac{\mathrm{d}x_k}{\mathrm{d}t}\right]}^{\mathrm{d}A_j/\mathrm{d}t}$$

$$= -q\left(\frac{\partial \phi}{\partial x_j} + \frac{\partial A_j}{\partial t}\right) + q\sum_k \frac{\mathrm{d}x_k}{\mathrm{d}t}\left[\frac{\partial A_k}{\partial x_j} - \frac{\partial A_j}{\partial x_k}\right] \qquad \textbf{(3.118.1)}$$

-- The first term on the right-hand side is just $-qE_j$:

$$\mathbf{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \mathbf{A}}{\partial t} \quad \Rightarrow \quad E_j = -\left(\frac{\partial \phi}{\partial x_j} + \frac{\partial A_j}{\partial t}\right)$$

The second term in (3.118.1) is, hopefully, the j'th component of

$$q(\mathbf{v} \wedge \mathbf{B}) = q\mathbf{v} \wedge (\boldsymbol{\nabla} \wedge \mathbf{A})$$

A : Classical Electrodynamics (5)

-- To check this :

$$(\mathbf{v} \wedge \mathbf{B})_j = \sum_{k,l} \epsilon_{jkl} v_k B_l = \sum_{k,l} \epsilon_{jkl} v_k \Big(\sum_{m,n} \epsilon_{lmn} \frac{\partial}{\partial x_m} A_n \Big)$$

-- Using the identity

$$\sum_{l} \epsilon_{jkl} \epsilon_{lmn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}$$

then gives

$$(\mathbf{v} \wedge \mathbf{B})_j = \sum_{k,m,n} (\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) v_k \frac{\partial A_n}{\partial x_m}$$

$$= \sum_{n} v_n \frac{\partial A_n}{\partial x_j} - \sum_{m} v_m \frac{\partial A_j}{\partial x_m}$$

$$= \sum_{k} v_k \frac{\partial A_k}{\partial x_j} - \sum_{k} v_k \frac{\partial A_j}{\partial x_k}$$

which is indeed the second term in eqn. (3.118.1), with $v_k \equiv \dfrac{\mathrm{d}x_k}{\mathrm{d}t}$

A : Classical Electrodynamics (6)

-- Hence equation (3.118.1) is the Lorentz force equation :

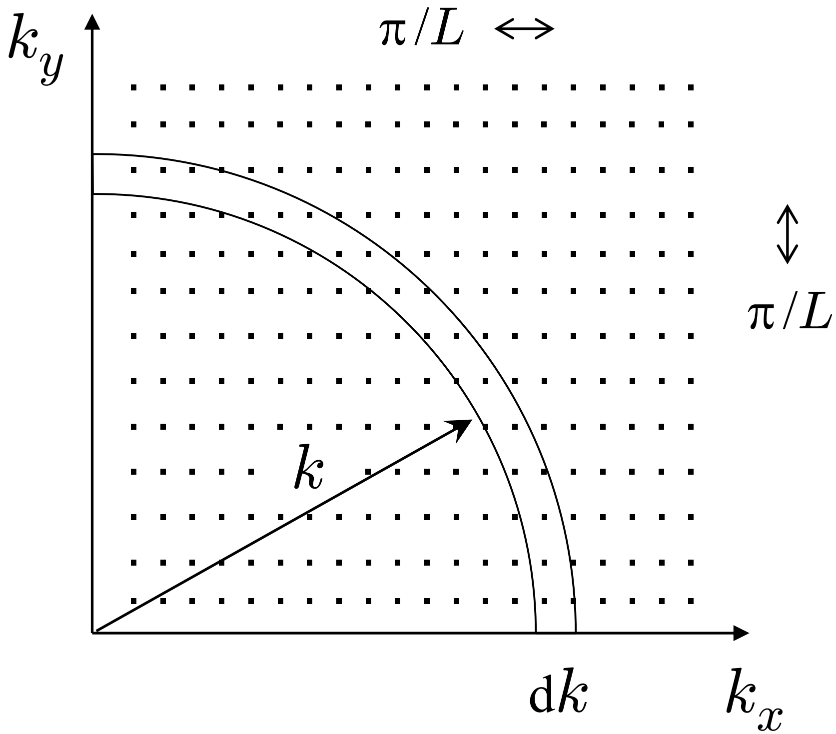
$$m\frac{\mathrm{d}^2 x_j}{\mathrm{d}t^2} = qE_j + q(\mathbf{v} \wedge \mathbf{B})_j \ ; \qquad \boxed{m\ddot{\mathbf{r}} = q\mathbf{E} + q\mathbf{v} \wedge \mathbf{B}}$$

B : Density of States

-- Consider a particle confined to the ***2D*** square region

$$0 < x < L\,, \quad 0 < y < L$$

-- If we impose "*hard wall*" boundary conditions, $\psi(\mathbf{r}) = 0$ on the sides of the square region, the allowed $\mathbf{k}$ vectors are (slide 1.38)



$$\mathbf{k} = (k_x, k_y) = \left(\frac{\pi n_x}{L}, \frac{\pi n_y}{L}\right)$$

$$n_x, n_y = 1, 2, 3, \ldots$$

The vector $\mathbf{k}$ is restricted to lie in the positive quadrant,

$$k_x > 0, \quad k_y > 0,$$

on a grid of points with grid spacing

$$\Delta k_x = \Delta k_y = \frac{\pi}{L}$$

B : Density of states : 2D (2)

-- In this case, the number of states $\mathrm{d}N$ with wavenumber between k and $k + \mathrm{d}k$ is obtained by counting states within one quarter of an annulus :

$$\mathrm{d}N = \frac{1}{4} \times \frac{2\pi k\,\mathrm{d}k}{(\pi/L)^2} = \frac{kL^2}{2\pi}\,\mathrm{d}k \qquad (k = |\mathbf{k}|)$$

-- Alternatively, we can restrict the available states by imposing *periodic* boundary conditions in the x and y directions :

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

In this case, the allowed states are separated in 2D $\mathbf{k}$-space by intervals

$$\Delta k_x = \Delta k_y = 2\pi/L$$

and $\mathbf{k}$ is no longer restricted to a single quadrant (k_x and k_y can be of either sign)

-- This gives the same number of states $\mathrm{d}N$ as for hard-wall b.c.'s :

$$\mathrm{d}N = \frac{2\pi k\,\mathrm{d}k}{(2\pi/L)^2} = \frac{kL^2}{2\pi}\,\mathrm{d}k$$

B : Density of states : 2D (3)

-- For a non-relativistic particle of mass m, the density of states can be converted from wavenumber k to energy E using

$$E = \frac{\hbar^2 k^2}{2m} \; ; \qquad \frac{\mathrm{d}N}{\mathrm{d}E} = \frac{\mathrm{d}N}{\mathrm{d}k}\frac{\mathrm{d}k}{\mathrm{d}E} = \frac{kL^2}{2\pi}\frac{m}{\hbar^2 k} = \frac{L^2 m}{2\pi\hbar^2}$$

The density of states per unit area, $g(E) = (\mathrm{d}N/\mathrm{d}E)/L^2$, is therefore

$$\boxed{g(E) = \frac{m}{2\pi\hbar^2}}$$

Thus, in 2D, $g(E)$ is in fact a constant, independent of energy

-- The density of states above applies to spin-zero particles

For spin-half particles, for example, an extra factor of two is needed to account for the spin degrees of freedom :

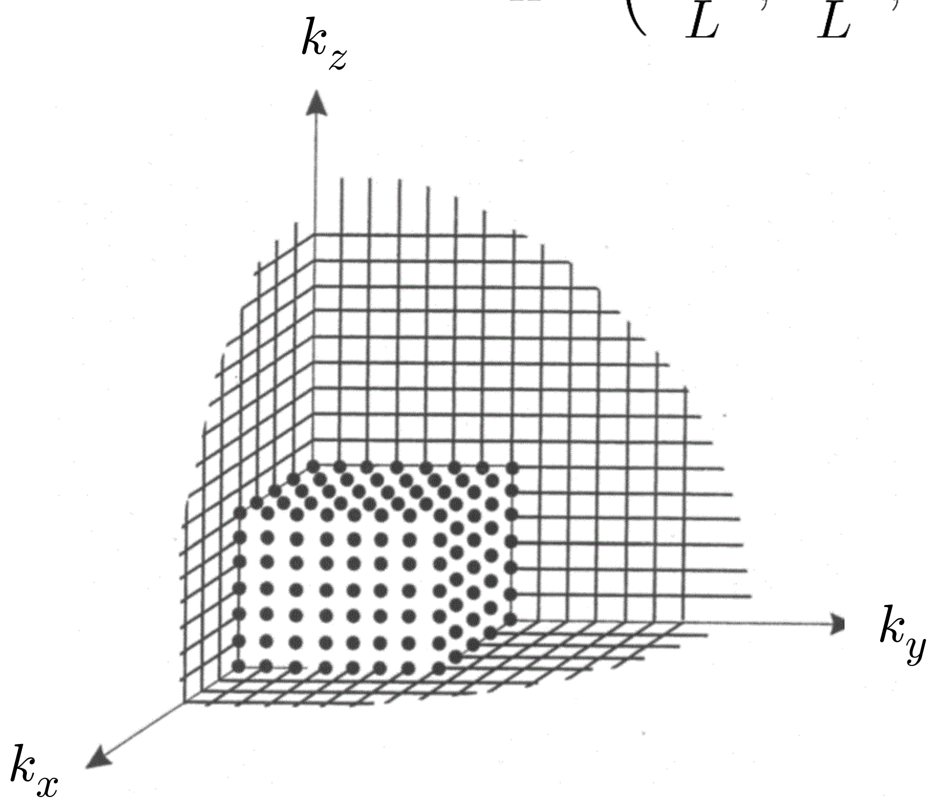
$$g(E) = \frac{m}{\pi\hbar^2}$$

B : Density of states : 3D

-- In ***3D***, we calculate the density of states $g(E)$ by considering a particle confined within a cubical box of side L :

Imposing hard-wall boundary conditions $\psi(\mathbf{r}) = 0$ on the sides of the box restricts the allowed $\mathbf{k}$ vector components to be

$$\mathbf{k} = \left(\frac{\pi n_x}{L}, \frac{\pi n_y}{L}, \frac{\pi n_z}{L} \right) \quad ; \qquad n_x, n_y, n_z = 1, 2, 3, \ldots$$



The vector $\mathbf{k}$ is restricted to lie in the positive octant,

$$k_x > 0, \quad k_y > 0, \quad k_z > 0,$$

on a grid of points with grid spacing

$$\Delta k_x = \Delta k_y = \Delta k_z = \frac{\pi}{L}$$

B : Density of states : 3D (2)

-- The number of available states $\mathrm{d}N$ between k and $k+\mathrm{d}k$ is obtained by counting states within one octant of a spherical shell :

$$\mathrm{d}N = \frac{1}{8} \times \frac{4\pi k^2\,\mathrm{d}k}{(\pi/L)^3} = \frac{k^2L^3}{2\pi^2}\,\mathrm{d}k \qquad (k = |\mathbf{k}|)$$

-- The same result can be obtained by imposing periodic instead of hard-wall boundary conditions :

$$\mathrm{d}N = \frac{4\pi k^2\,\mathrm{d}k}{(2\pi/L)^3} = \frac{k^2L^3}{2\pi^2}\,\mathrm{d}k$$

-- For a non-relativistic particle of mass m, the number of states per unit energy is

$$\frac{\mathrm{d}N}{\mathrm{d}E} = \frac{\mathrm{d}N}{\mathrm{d}k}\frac{\mathrm{d}k}{\mathrm{d}E} = \frac{k^2L^3}{2\pi^2}\frac{m}{\hbar^2 k} = \frac{L^3mk}{2\pi^2\hbar^2}$$

The density of states per unit volume is therefore proportional to $\sqrt{E}$:

$$\boxed{g(E) = \frac{mk}{2\pi^2\hbar^2}\ ; \qquad k = \frac{\sqrt{2mE}}{\hbar}}$$

B : Density of states : 3D (3)

-- For a (relativistic) *massless* particle such as a photon, with energy

$$E = \hbar\omega(\mathbf{k}) = \hbar c k$$

the conversion from k to E becomes

$$\frac{\mathrm{d}N}{\mathrm{d}E} = \frac{\mathrm{d}N}{\mathrm{d}k}\frac{\mathrm{d}k}{\mathrm{d}E} = \frac{k^2 L^3}{2\pi^2}\frac{1}{\hbar c} = \frac{L^3}{2\pi^2(\hbar c)^3}E^2$$

The density of states per unit volume is therefore proportional to E^2 :

$$\boxed{g(E) = \frac{E^2}{2\pi^2(\hbar c)^3}} \qquad (m = 0)$$

-- Additional factors may be needed to take spin degrees of freedom into account (an extra factor of two for photons, for example)

B : Density of states : 3D (4)

-- For particles whose direction of motion is restricted to lie within a solid angle $\Delta\Omega$, an extra factor $\Delta\Omega/4\pi$ is needed :

For a non-relativistic particle of mass m, the density of states (per unit volume, per spin degree of freedom) within $\Delta\Omega$ is

$$g(E) = \frac{mk}{2\pi^2\hbar^2} \times \frac{\Delta\Omega}{4\pi} = \frac{mk}{8\pi^3\hbar^2}\Delta\Omega \; ; \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

For a massless particle, we obtain instead

$$g(E) = \frac{E^2}{2\pi^2(\hbar c)^3} \times \frac{\Delta\Omega}{4\pi} = \frac{E^2}{(2\pi\hbar c)^3}\,\Delta\Omega \qquad (m = 0)$$