Chapter 5

Motion of a charged particle in a magnetic field

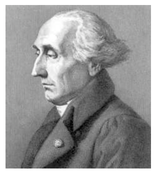
Hitherto, we have focussed on applications of quantum mechanics to free particles or particles confined by scalar potentials. In the following, we will address the influence of a magnetic field on a charged particle. Classically, the force on a charged particle in an electric and magnetic field is specified by the **Lorentz force law**:

$$\mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) ,$$

where q denotes the charge and $\mathbf{v}$ the velocity. (Here we will adopt a convention in which q denotes the charge (which may be positive or negative) and $e \equiv |e|$ denotes the *modulus* of the electron charge, i.e. for an electron, the charge $q = -e = -1.602176487 \times 10^{-19}$ C.) The velocity-dependent force associated with the magnetic field is quite different from the conservative forces associated with scalar potentials, and the programme for transferring from classical to quantum mechanics - replacing momenta with the appropriate operators - has to be carried out with more care. As preparation, it is helpful to revise how the Lorentz force arises in the Lagrangian formulation of classical mechanics.

Hendrik Antoon Lorentz 1853-1928
A Dutch physicist who shared the 1902 Nobel Prize in Physics with Pieter Zeeman for the discovery and theoretical explanation of the Zeeman effect. He also derived the transformation equations subsequently used by Albert Einstein to describe space and time.

Joseph-Louis Lagrange, born Giuseppe Lodovico Lagrangia 1736-1813
An Italian-born mathematician and astronomer, who lived most of his life in Prussia and France, making significant contributions to all fields of analysis, to number theory, and to classical and celestial mechanics. On the recommendation of Euler and D'Alembert, in 1766 Lagrange succeeded Euler as the director of mathematics at the Prussian Academy of Sciences in Berlin, where he stayed for over twenty years, producing a large body of work and winning several prizes of the French Academy of Sciences. Lagrange's treatise on analytical mechanics, written in Berlin and first published in 1788, offered the most comprehensive treatment of classical mechanics since Newton and formed a basis for the development of mathematical physics in the nineteenth century.



5.1 Classical mechanics of a particle in a field

For a system with m degrees of freedom specified by coordinates $q_1, \cdots q_m$, the classical action is determined from the Lagrangian $L(q_i, \dot{q}_i)$ by

$$\boxed{S[q_i] = \int dt\, L(q_i, \dot{q}_i)\,.}$$

The action is said to be a **functional** of the coordinates $q_i(t)$. According to **Hamilton's extremal principle** (also known as the **principle of least action**), the dynamics of a classical system is described by the equations that minimize the action. These equations of motion can be expressed through the classical Lagrangian in the form of the Euler-Lagrange equations,

$$\boxed{\frac{d}{dt}(\partial_{\dot{q}_i} L(q_i, \dot{q}_i)) - \partial_{q_i} L(q_i, \dot{q}_i) = 0\,.} \tag{5.1}$$

▷ Info. **Euler-Lagrange equations:** According to Hamilton's extremal principle, for any smooth set of curves $w_i(t)$, the variation of the action around the classical solution $q_i(t)$ is zero, i.e. $\lim_{\epsilon\to 0} \frac{1}{\epsilon}(S[q_i + \epsilon w_i] - S[q_i]) = 0$. Applied to the action, the variation implies that, for any i, $\int dt\,(w_i \partial_{q_i} L(q_i, \dot{q}_i) + \dot{w}_i \partial_{\dot{q}_i} L(q_i, \dot{q}_i)) = 0$. Then, integrating the second term by parts, and droping the boundary term, one obtains

$$\int dt\, w_i \left(\partial_{q_i} L(q_i, \dot{q}_i) - \frac{d}{dt}\partial_{\dot{q}_i} L(q_i, \dot{q}_i)\right) = 0\,.$$

Since this equality must follow for any function $w_i(t)$, the term in parentheses in the integrand must vanish leading to the Euler-Lagrange equation (5.1).

The **canonical momentum** is specified by the equation $p_i = \partial_{\dot{q}_i} L$, and the classical Hamiltonian is defined by the Legendre transform,

$$\boxed{H(q_i, p_i) = \sum_i p_i q_i - L(q_i, \dot{q}_i)\,.} \tag{5.2}$$

It is straightforward to check that the equations of motion can be written in the form of Hamilton's equations of motion,

$$\boxed{\dot{q}_i = \partial_{p_i} H, \qquad \dot{p}_i = -\partial_{q_i} H\,.}$$

Siméon Denis Poisson 1781-1840
A French mathematician, geometer, and physicist whose mathematical skills enabled him to compute the distribution of electrical charges on the surface of conductors. He extended the work of his mentors, Pierre Simon Laplace and Joseph Louis Lagrange, in celestial mechanics by taking their results to a higher order of accuracy. He was also known for his work in probability.

From these equations it follows that, if the Hamiltonian is independent of a particular coordinate q_i, the corresponding momentum p_i remains constant. For **conservative forces**,[1] the classical Lagrangian and Hamiltonian can be written as $L = T - V$, $H = T + V$, with T the kinetic energy and V the potential energy.

▷ INFO. **Poisson brackets:** Any dynamical variable f in the system is some function of the phase space coordinates, the q_is and p_is, and (assuming it does not depend explicitly on time) its time-development is given by:

$$\frac{d}{dt} f(q_i, p_i) = \partial_{q_i} f\, \dot{q}_i + \partial_{p_i} f\, \dot{p}_i = \partial_{q_i} f\, \partial_{p_i} H - \partial_{p_i} f\, \partial_{q_i} H \equiv \{f, H\}.$$

The curly brackets are known as Poisson brackets, and are defined for any dynamical variables as $\{A, B\} = \partial_{q_i} A\, \partial_{p_i} B - \partial_{p_i} A\, \partial_{q_i} B$. From Hamilton's equations, we have shown that for any variable, $\dot{f} = \{f, H\}$. It is easy to check that, for the coordinates and canonical momenta, $\{q_i, q_j\} = 0 = \{p_i, p_j\}, \qquad \{q_i, p_j\} = \delta_{ij}$. This was the classical mathematical structure that led Dirac to link up classical and quantum mechanics: He realized that the Poisson brackets were the classical version of the commutators, so a classical canonical momentum must correspond to the quantum differential operator in the corresponding coordinate.[2]

With these foundations revised, we now return to the problem at hand; the infleunce of an electromagnetic field on the dynamics of the charged particle.

As the Lorentz force is velocity dependent, it can not be expressed simply as the gradient of some potential. Nevertheless, the classical path traversed by a charged particle is still specifed by the principle of least action. The electric and magnetic fields can be written in terms of a scalar and a vector potential as $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\nabla\phi - \dot{\mathbf{A}}$. The corresponding Lagrangian takes the form:[3]

$$L = \frac{1}{2} m \mathbf{v}^2 - q\phi + q\mathbf{v}\cdot\mathbf{A}.$$

[1] i.e. forces that conserve mechanical energy.

[2] For a detailed discussion, we refer to Paul A. M. Dirac, *Lectures on Quantum Mechanics*, Belfer Graduate School of Science Monographs Series Number 2, 1964.

[3] In a relativistic formulation, the interaction term here looks less arbitrary: the relativistic version would have the relativistically invariant $q\int A^\mu dx_\mu$ added to the action integral, where the four-potential $A_\mu = (\phi, \mathbf{A})$ and $dx_\mu = (ct, dx_1, dx_2, dx_3)$. This is the simplest possible invariant interaction between the electromagnetic field and the particle's four-velocity. Then, in the non-relativistic limit, $q\int A^\mu dx_\mu$ just becomes $q\int(\mathbf{v}\cdot\mathbf{A} - \phi)dt$.

In this case, the general coordinates $q_i \equiv x_i = (x_1, x_2, x_3)$ are just the Cartesian coordinates specifying the position of the particle, and the $\dot{q}_i$ are the three components $\dot{x}_i = (\dot{x}_1, \dot{x}_2, \dot{x}_3)$ of the particle velocities. The important point is that the *canonical* momentum

$$p_i = \partial_{\dot{x}_i} L = m v_i + q A_i \,,$$

is no longer simply given by the mass × velocity – there is an extra term!

Making use of the definition (5.2), the corresponding Hamiltonian is given by

$$H(q_i, p_i) = \sum_i (m v_i + q A_i)\, v_i - \frac{1}{2} m \mathbf{v}^2 + q\phi - q\mathbf{v}\cdot\mathbf{A} = \frac{1}{2} m\mathbf{v}^2 + q\phi \,.$$

Reassuringly, the Hamiltonian just has the familiar form of the sum of the kinetic and potential energy. However, to get Hamilton's equations of motion, the Hamiltonian has to be expressed solely in terms of the coordinates and canonical momenta, i.e.

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

Let us now consider Hamilton's equations of motion, $\dot{x}_i = \partial_{p_i} H$ and $\dot{p}_i = -\partial_{x_i} H$. The first equation recovers the expression for the canonical momentum while second equation yields the Lorentz force law. To understand how, we must first keep in mind that dp/dt is not the acceleration: The A-dependent term also varies in time, and in a quite complicated way, since it is the field at a point moving with the particle. More precisely,

$$\dot{p}_i = m\ddot{x}_i + q\dot{A}_i = m\ddot{x}_i + q\left(\partial_t A_i + v_j \partial_{x_j} A_i\right) \,,$$

where we have assumed a summation over repeated indicies. The right-hand side of the second of Hamilton's equation, $\dot{p}_i = -\frac{\partial H}{\partial x_i}$, is given by

$$-\partial_{x_i} H = \frac{1}{m}(\mathbf{p} - q\mathbf{A}(\mathbf{r}, t)) q\partial_{x_i}\mathbf{A} - q\partial_{x_i}\phi(\mathbf{r}, t) = q v_j \partial_{x_i} A_j - q\partial_{x_i}\phi \,.$$

Together, we obtain the equation of motion, $m\ddot{x}_i = -q\left(\partial_t A_i + v_j \partial_{x_j} A_i\right) + q v_j \partial_{x_i} A_j - q\partial_{x_i}\phi$. Using the identity, $\mathbf{v}\times(\nabla\times\mathbf{A}) = \nabla(\mathbf{v}\cdot\mathbf{A}) - (\mathbf{v}\cdot\nabla)\mathbf{A}$, and the expressions for the electric and magnetic fields in terms of the potentials, one recovers the Lorentz equations

$$m\ddot{x} = \mathbf{F} = q\left(\mathbf{E} + \mathbf{v}\times\mathbf{B}\right) \,.$$

With these preliminary discussions of the classical system in place, we are now in a position to turn to the quantum mechanics.

5.2 Quantum mechanics of a particle in a field

To transfer to the quantum mechanical regime, we must once again implement the canonical quantization procedure setting $\hat{\mathbf{p}} = -i\hbar\nabla$, so that $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$. However, in this case, $\hat{p}_i \neq m\hat{v}_i$. This leads to the novel situation that the velocities in different directions do not commute.[4] To explore influence of the magnetic field on the particle dynamics, it is helpful to assess the relative weight of the $\mathbf{A}$-dependent contributions to the quantum Hamiltonian,

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

[4]With $m\hat{v}_i = -i\hbar\partial_{x_i} - qA_i$, it is easy (and instructive) to verify that $[\hat{v}_x, \hat{v}_y] = \frac{i\hbar q}{m^2} B$.

Expanding the square on the right hand side of the Hamiltonian, the cross-term (known as the **paramagnetic term**) leads to the contribution $-\frac{q\hbar}{2im}(\nabla\cdot\mathbf{A}+\mathbf{A}\cdot\nabla) = \frac{iq\hbar}{m}\mathbf{A}\cdot\nabla$, where the last equality follows from the Coulomb gauge condition, $\nabla\cdot\mathbf{A}=0$.[5] Combined with the **diamagnetic** ($\mathbf{A}^2$) contribution, one obtains the Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{iq\hbar}{m}\mathbf{A}\cdot\nabla + \frac{q^2}{2m}\mathbf{A}^2 + q\phi\,.$$

For a constant magnetic field, the vector potential can be written as $\mathbf{A} = -\mathbf{r}\times\mathbf{B}/2$. In this case, the paramagnetic component takes the form

$$\frac{iq\hbar}{m}\mathbf{A}\cdot\nabla = \frac{iq\hbar}{2m}(\mathbf{r}\times\nabla)\cdot\mathbf{B} = -\frac{q}{2m}\mathbf{L}\cdot\mathbf{B}\,,$$

where $\mathbf{L}$ denotes the angular momentum operator (with the hat not shown for brevity!). Similarly, the diamagnetic term leads to

$$\frac{q^2}{2m}\mathbf{A}^2 = \frac{q^2}{8m}\left(\mathbf{r}^2\mathbf{B}^2 - (\mathbf{r}\cdot\mathbf{B})^2\right) = \frac{q^2B^2}{8m}(x^2+y^2)\,,$$

where, here, we have chosen the magnetic field to lie along the z-axis.

5.3 Atomic hydrogen: Normal Zeeman effect

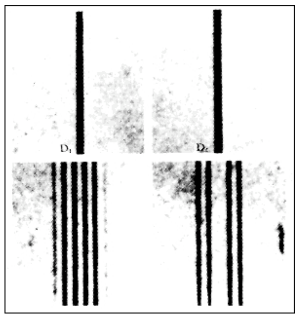
Before addressing the role of these separate contributions in atomic hydrogen, let us first estimate their relative magnitude. With $\langle x^2+y^2\rangle \simeq a_0^2$, where a_0 denotes the Bohr radius, and $\langle L_z\rangle \simeq \hbar$, the ratio of the paramagnetic and diamagnetic terms is given by

$$\frac{(q^2/8m_e)\langle x^2+y^2\rangle B^2}{(q/2m_e)\langle L_z\rangle B} = \frac{e}{4}\frac{a_0^2B^2}{\hbar B} \simeq 10^{-6}\,B/\mathrm{T}\,.$$

Therefore, while electrons remain bound to atoms, for fields that can be achieved in the laboratory ($B \simeq 1\,\mathrm{T}$), the diamagnetic term is negligible as compared to the paramagnetic term. Moreover, when compared with the Coulomb energy scale,

$$\frac{eB\hbar/2m_e}{m_ec^2\alpha^2/2} = \frac{e\hbar}{(m_ec\alpha)^2}B \simeq \frac{B/\mathrm{T}}{2.3\times10^5}\,,$$

where $\alpha = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c} \simeq \frac{1}{137}$ denotes the fine structure constant, one may see that the paramagnetic term provides only a small perturbation to the typical atomic splittings.



Splitting of the sodium D lines due to an external magnetic field. The multiplicity of the lines and their "selection rule" will be discussed more fully in chapter 9. The figure is taken from the original paper, P. Zeeman, *The effect of magnetization on the nature of light emitted by a substance*, Nature **55**, 347 (1897).

[5]The electric field $\mathbf{E}$ and magnetic field $\mathbf{B}$ of Maxwell's equations contain only "physical" degrees of freedom, in the sense that every mathematical degree of freedom in an electromagnetic field configuration has a separately measurable effect on the motions of test charges in the vicinity. As we have seen, these "field strength" variables can be expressed in terms of the scalar potential ϕ and the vector potential $\mathbf{A}$ through the relations: $\mathbf{E} = -\nabla\phi - \partial_t\mathbf{A}$ and $\mathbf{B} = \nabla\times\mathbf{A}$. Notice that if $\mathbf{A}$ is transformed to $\mathbf{A}+\nabla\Lambda$, $\mathbf{B}$ remains unchanged, since $\mathbf{B} = \nabla\times[\mathbf{A}+\nabla\Lambda] = \nabla\times\mathbf{A}$. However, this transformation changes $\mathbf{E}$ as

$$\mathbf{E} = -\nabla\phi - \partial_t\mathbf{A} - \nabla\partial_t\Lambda = -\nabla[\phi+\partial_t\Lambda] - \partial_t\mathbf{A}\,.$$

If ϕ is further changed to $\phi - \partial_t\Lambda$, $\mathbf{E}$ remains unchanged. Hence, both the $\mathbf{E}$ and $\mathbf{B}$ fields are unchanged if we take any function $\Lambda(\mathbf{r},t)$ and simultaneously transform

$$\mathbf{A} \to \mathbf{A} + \nabla\Lambda$$
$$\phi \to \phi - \partial_t\Lambda\,.$$

A particular choice of the scalar and vector potentials is a **gauge**, and a scalar function Λ used to change the gauge is called a gauge function. The existence of arbitrary numbers of gauge functions $\Lambda(\mathbf{r},t)$, corresponds to the U(1) gauge freedom of the theory. Gauge fixing can be done in many ways.

However, there are instances when the diamagnetic contriubution can play an important role. Leaving aside the situation that may prevail on neutron stars, where magnetic fields as high as 10^8 T may exist, the diamagnetic contribution can be large when the typical "orbital" scale $\langle x^2 + y^2\rangle$ becomes macroscopic in extent. Such a situation arises when the electrons become unbound such as, for example, in a metal or a synchrotron. For a further discussion, see section 5.5 below.

Retaining only the paramagnetic contribution, the Hamiltonian for a "spinless" electron moving in a Coulomb potential in the presence of a constant magnetic field then takes the form,

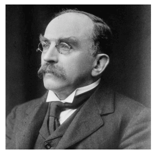
$$\hat{H} = \hat{H}_0 + \frac{e}{2m} B L_z\,,$$

where $\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}$. Since $[\hat{H}_0, L_z] = 0$, the eigenstates of the unperturbed Hamiltonian, $\psi_{l\ell m}(\mathbf{r})$ remain eigenstates of $\hat{H}$ and the corresponding energy levels are specified by

$$E_{n\ell m} = -\frac{\mathrm{Ry}}{n^2} + \hbar\omega_{\mathrm{L}} m$$

where $\omega_{\mathrm{L}} = \frac{eB}{2m}$ denotes the **Larmor frequency**. From this result, we expect that a constant magnetic field will lead to a splitting of the $(2\ell+1)$-fold degeneracy of the energy levels leading to multiplets separated by a constant energy shift of $\hbar\omega_{\mathrm{L}}$. The fact that this behaviour is not recapitulated generically by experiment was one of the key insights that led to the identification of electron spin, a matter to which we will turn in chapter 6.

Sir Joseph Larmor 1857-1942
A physicist and mathematician who made innovations in the understanding of electricity, dynamics, thermodynamics, and the electron theory of matter. His most influential work was *Aether and Matter*, a theoretical physics book published in 1900. In 1903 he was appointed Lucasian Professor of Mathematics at Cambridge, a post he retained until his retirement in 1932.



5.4 Gauge invariance and the Aharonov-Bohm effect

Our derivation above shows that the quantum mechanical Hamiltonian of a charged particle is defined in terms of the vector potential, $\mathbf{A}$. Since the latter is defined only up to some gauge choice, this suggests that the wavefunction is not a gauge invariant object. Indeed, it is only the observables associated with the wavefunction which must be gauge invariant. To explore this gauge freedom, let us consider the influence of the **gauge transformation**,

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad \phi \mapsto \phi' - \partial_t\Lambda\,,$$

where $\Lambda(\mathbf{r}, t)$ denotes a scalar function. Under the gauge transformation, one may show that the corresponding wavefunction gets transformed as

$$\psi'(\mathbf{r}, t) = \exp\left[i\frac{q}{\hbar}\Lambda(\mathbf{r}, t)\right]\psi(\mathbf{r}, t)\,. \tag{5.3}$$

▷ Exercise. If wavefunction $\psi(\mathbf{r}, t)$ obeys the time-dependent Schrödinger equation, $i\hbar\partial_t\psi = \hat{H}[\mathbf{A}, \phi]\psi$, show that $\psi'(\mathbf{r}, t)$ as defined by (5.3) obeys the equation $i\hbar\partial_t\psi' = \hat{H}'[\mathbf{A}', \phi']\psi'$.

The gauge transformation introduces an additional space and time-dependent phase factor into the wavefunction. However, since the observable translates to the probability density, $|\psi|^2$, this phase dependence seems invisible.

▷ Info. One physical manifestation of the gauge invariance of the wavefunction is found in the **Aharonov-Bohm effect**. Consider a particle with charge q travelling

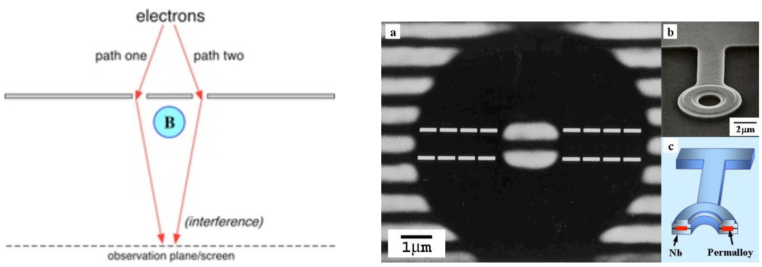


Figure 5.1: (Left) Schematic showing the geometry of an experiment to observe the Aharonov-Bohm effect. Electrons from a coherent source can follow two paths which encircle a region where the magnetic field is non-zero. (Right) Interference fringes for electron beams passing near a toroidal magnet from the experiment by Tonomura and collaborators in 1986. The electron beam passing through the center of the torus acquires an additional phase, resulting in fringes that are shifted with respect to those outside the torus, demonstrating the Aharonov-Bohm effect. For details see the original paper from which this image was borrowed see Tonomura *et al.*, *Evidence for Aharonov-Bohm effect with magnetic field completely shielded from electron wave*, Phys. Rev. Lett. **56**, 792 (1986).

along a path, P, in which the magnetic field, $\mathbf{B} = 0$ is identically zero. However, a vanishing of the magnetic field does not imply that the vector potential, $\mathbf{A}$ is zero. Indeed, as we have seen, any $\Lambda(\mathbf{r})$ such that $\mathbf{A} = \nabla\Lambda$ will translate to this condition. In traversing the path, the wavefunction of the particle will acquire the phase factor $\varphi = \frac{q}{\hbar}\int_P \mathbf{A}\cdot d\mathbf{r}$, where the line integral runs along the path.

If we consider now two separate paths P and P' which share the same initial and final points, the relative phase of the wavefunction will be set by

$$\Delta\varphi = \frac{q}{\hbar}\int_P \mathbf{A}\cdot d\mathbf{r} - \frac{q}{\hbar}\int_{P'} \mathbf{A}\cdot d\mathbf{r} = \frac{q}{\hbar}\oint \mathbf{A}\cdot d\mathbf{r} = \frac{q}{\hbar}\int_A \mathbf{B}\cdot d^2\mathbf{r}\,,$$

where the line integral $\oint$ runs over the loop involving paths P and P', and $\int_A$ runs over the area enclosed by the loop. The last relation follows from the application of Stokes' theorem. This result shows that the relative phase $\Delta\varphi$ is fixed by the factor $q/\hbar$ multiplied by the magnetic flux $\Phi = \int_A \mathbf{B}\cdot d^2\mathbf{r}$ enclosed by the loop.[6] In the absence of a magnetic field, the flux vanishes, and there is no additional phase.

However, if we allow the paths to enclose a region of non-vanishing magnetic field (see figure 5.1(left)), *even if the field is identically zero on the paths P and P'*, the wavefunction will acquire a non-vanishing relative phase. This flux-dependent phase difference translates to an observable shift of interference fringes when on an observation plane. Since the original proposal,[7] the Aharonov-Bohm effect has been studied in several experimental contexts. Of these, the most rigorous study was undertaken by Tonomura in 1986. Tomomura fabricated a doughnut-shaped (toroidal) ferromagnet six micrometers in diameter (see figure 5.1b), and covered it with a niobium superconductor to completely confine the magnetic field within the doughnut, in accordance with the Meissner effect.[8] With the magnet maintained at 5 K, they measured the phase difference from the interference fringes between one electron beam passing though the hole in the doughnut and the other passing on the outside of the doughnut. The results are shown in figure 5.1(right,a). Interference fringes are displaced with just half a fringe of spacing inside and outside of the doughnut, indicating the existence of the Aharonov-Bohm effect. Although electrons pass through regions free of any electromagnetic field, an observable effect was produced due to the existence of vector potentials.

Sir George Gabriel Stokes, 1st Baronet 1819-1903

A mathematician and physicist, who at Cambridge made important contributions to fluid dynamics (including the NavierStokes equations), optics, and mathematical physics (including Stokes' theorem). He was secretary, and then president, of the Royal Society.

[6] Note that the phase difference depends on the magnetic flux, a function of the magnetic field, and is therefore a gauge invariant quantity.

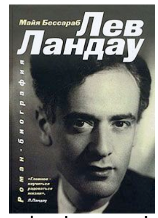
[7] Y. Aharonov and D. Bohm, *Significance of electromagnetic potentials in quantum theory*, Phys. Rev. **115**, 485 (1959).

[8] Perfect diamagnetism, a hallmark of superconductivity, leads to the complete expulsion of magnetic fields – a phenomenon known as the Meissner effect.

The observation of the half-fringe spacing reflects the constraints imposed by the superconducting toroidal shield. When a superconductor completely surrounds a magnetic flux, the flux is quantized to an integral multiple of quantized flux $h/2e$, the factor of two reflecting that fact that the superconductor involves a condensate of electron *pairs*. When an odd number of vortices are enclosed inside the superconductor, the relative phase shift becomes π (mod. 2π) – half-spacing! For an even number of vortices, the phase shift is zero.[9]

5.5 Free electrons in a magnetic field: Landau levels

Lev Davidovich Landau 1908-1968



A prominent Soviet physicist who made fundamental contributions to many areas of theoretical physics. His accomplishments include the co-discovery of the density matrix method in quantum mechanics, the quantum mechanical theory of diamagnetism, the theory of superfluidity, the theory of second order phase transitions, the Ginzburg-Landau theory of superconductivity, the explanation of Landau damping in plasma physics, the Landau pole in quantum electrodynamics, and the two-component theory of neutrinos. He received the 1962 Nobel Prize in Physics for his development of a mathematical theory of superfluidity that accounts for the properties of liquid helium II at a temperature below 2.17K.

Finally, to complete our survey of the influence of a uniform magnetic field on the dynamics of charged particles, let us consider the problem of a free quantum particle. In this case, the classical electron orbits can be macroscopic and there is no reason to neglect the diamagnetic contribution to the Hamiltonian. Previously, we have worked with a gauge in which $\mathbf{A} = (-y, x, 0)B/2$, giving a constant field B in the z-direction. However, to address the Schrödinger equation for a particle in a uniform perpendicular magnetic field, it is convenient to adopt the **Landau gauge**, $\mathbf{A}(\mathbf{r}) = (-By, 0, 0)$.

▷ EXERCISE. Construct the gauge transformation, $\Lambda(\mathbf{r})$ which connects these two representations of the vector potential.

In this case, the stationary form of the Schrödinger equation is given by

$$\hat{H}\psi(\mathbf{r}) = \frac{1}{2m}\left[(\hat{p}_x + qBy)^2 + \hat{p}_y^2 + \hat{p}_z^2\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})\,.$$

Since $\hat{H}$ commutes with both $\hat{p}_x$ and $\hat{p}_z$, both operators have a common set of eigenstates reflecting the fact that p_x and p_z are conserved by the dynamics. The wavefunction must therefore take the form, $\psi(\mathbf{r}) = e^{i(p_x x + ip_z z)/\hbar}\chi(y)$, with $\chi(y)$ defined by the equation,

$$\left[\frac{\hat{p_y}^2}{2m} + \frac{1}{2}m\omega^2(y - y_0)^2\right]\chi(y) = \left(E - \frac{p_z^2}{2m}\right)\chi(y)\,.$$

Here $y_0 = -p_x/qB$ and $\omega = |q|B/m$ coincides with the **cyclotron frequency** of the classical charged particle (exercise). We now see that the conserved canonical momentum p_x in the x-direction is in fact the coordinate of the centre of a simple harmonic oscillator potential in the y-direction with frequency ω. As a result, we can immediately infer that the eigenvalues of the Hamiltonian are comprised of a free particle component associated with motion parallel to the field, and a set of harmonic oscillator states,

$$E_{n,p_z} = (n + 1/2)\hbar\omega + \frac{p_z^2}{2m}\,.$$

The quantum numbers, n, specify states known as **Landau levels**.

Let us confine our attention to states corresponding to the lowest oscillator (Landau level) state, (and, for simplicity, $p_z = 0$), $E_0 = \hbar\omega/2$. What is the degeneracy of this Landau level? Consider a rectangular geometry of area $A = L_x \times L_y$ and, for simplicity, take the boundary conditions to be periodic. The centre of the oscillator wavefunction, $y_0 = -p_x/qB$, must lie

[9]The superconducting flux quantum was actually predicted prior to Aharonov and Bohm, by Fritz London in 1948 using a phenomenological theory.

between 0 and L_y. With periodic boundary conditions $e^{ip_xL_x/\hbar} = 1$, so that $p_x = n2\pi\hbar/L_x$. This means that y_0 takes a series of evenly-spaced discrete values, separated by $\Delta y_0 = h/qBL_x$. So, for electron degrees of freedom, $q = -e$, the total number of states $N = L_y/|\Delta y_0|$, i.e.

$$\nu_{\max} = \frac{L_xL_y}{h/eB} = A\frac{B}{\Phi_0}\,, \tag{5.4}$$

where $\Phi_0 = e/h$ denotes the "flux quantum". So the total number of states in the lowest energy level coincides with the total number of flux quanta making up the field B penetrating the area A.

The Landau level degeneracy, $\nu_{\max}$, depends on field; the larger the field, the more electrons can be fit into each Landau level. In the physical system, each Landau level is spin split by the Zeeman coupling, with (5.4) applying to one spin only. Finally, although we treated x and y in an asymmetric manner, this was merely for convenience of calculation; no physical quantity should dierentiate between the two due to the symmetry of the original problem.

Klaus von Klitzing, 1943-

German physicist who was awarded the Nobel Prize for Physics in 1985 for his discovery that under appropriate conditions the resistance offered by an electrical conductor is quantized. The work was first reported in the following reference, K. v. Klitzing, G. Dorda, and M. Pepper, *New method for high-accuracy determination of the fine-structure constant based on quantized Hall resistance*, Phys. Rev. Lett. **45**, 494 (1980).

▷ Exercise. Consider the solution of the Schrödinger equation when working in the symmetric gauge with $\mathbf{A} = -\mathbf{r}\times\mathbf{B}/2$. Hint: consider the velocity commutation relations, $[v_x, v_y]$ and how these might be deployed as conjugate variables.

▷ Info. It is instructive to infer y_0 from purely classical considerations: Writing $m\dot{\mathbf{v}} = q\mathbf{v}\times\mathbf{B}$ in component form, we have $m\ddot{x} = \frac{qB}{c}\dot{y}$, $m\ddot{y} = -\frac{qB}{c}\dot{x}$, and $m\ddot{z} = 0$. Focussing on the motion in the xy-plane, these equations integrate straightforwardly to give, $m\dot{x} = \frac{qB}{c}(y - y_0)$, $m\dot{y} = -\frac{qB}{c}(x - x_0)$. Here (x_0, y_0) are the coordinates of the centre of the classical circular motion (known as the "**guiding centre**") – the velocity vector $\mathbf{v} = (\dot{x}, \dot{y})$ always lies perpendicular to $(\mathbf{r} - \mathbf{r}_0)$, and $\mathbf{r}_0$ is given by

$$y_0 = y - mv_x/qB = -p_x/qB, \qquad x_0 = x + mv_y/qB = x + p_y/qB\,.$$

(Recall that we are using the gauge $\mathbf{A}(x, y, z) = (-By, 0, 0)$, and $p_x = \partial_{\dot{x}}L = mv_x + qA_x$, etc.) Just as y_0 is a conserved quantity, so is x_0: it commutes with the Hamiltonian since $[x + c\hat{p}_y/qB, \hat{p}_x + qBy] = 0$. However, x_0 and y_0 do not commute with each other: $[x_0, y_0] = -i\hbar/qB$. This is why, when we chose a gauge in which y_0 was sharply defined, x_0 was spread over the sample. If we attempt to localize the point (x_0, y_0) as much as possible, it is smeared out over an area corresponding to one flux quantum. The natural length scale of the problem is therefore the magnetic length defined by $\ell = \sqrt{\frac{\hbar}{qB}}$.

▷ Info. **Integer quantum Hall effect:** Until now, we have considered the impact of just a magnetic field. Consider now the Hall effect geometry in which we apply a crossed electric, $\mathbf{E}$ and magnetic field, $\mathbf{B}$. Taking into account both contributions, the total current flow is given by

$$\mathbf{j} = \sigma_0\left(\mathbf{E} - \frac{\mathbf{j}\times\mathbf{B}}{ne}\right),$$

where σ_0 denotes the conductivity, and n is the electron density. With the electric field oriented along y, and the magnetic field along z, the latter equation may be rewritten as

$$\begin{pmatrix} 1 & \frac{\sigma_0 B}{ne} \\ -\frac{\sigma_0 B}{ne} & 1 \end{pmatrix}\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \sigma_0\begin{pmatrix} 0 \\ E_y \end{pmatrix}.$$

Inverting these equations, one finds that

$$j_x = \underbrace{\frac{-\sigma_0^2 B/ne}{1 + (\sigma_0 B/ne)^2}}_{\sigma_{xy}} E_y, \qquad j_y = \underbrace{\frac{\sigma_0}{1 + (\sigma_0 B/ne)^2}}_{\sigma_{yy}} E_y\,.$$

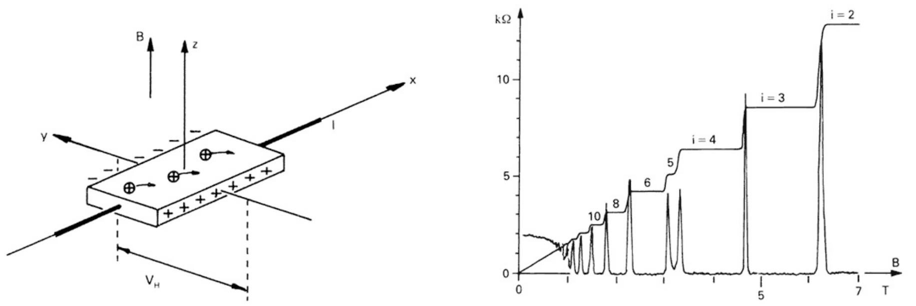


Figure 5.2: (Left) A voltage V drives a current I in the positive x direction. Normal Ohmic resistance is V/I. A magnetic field in the positive z direction shifts positive charge carriers in the negative y direction. This generates a Hall potential and a Hall resistance (VH/I) in the y direction. (Right) The Hall resistance varies stepwise with changes in magnetic field B. Step height is given by the physical constant h/e^2 (value approximately $25\,\mathrm{k}\Omega$) divided by an integer i. The figure shows steps for $i = 2, 3, 4, 5, 6, 8$ and 10. The effect has given rise to a new international standard for resistance. Since 1990 this has been represented by the unit 1 klitzing, defined as the Hall resistance at the fourth step ($h/4e^2$). The lower peaked curve represents the Ohmic resistance, which disappears at each step.

These provide the classical expressions for the longitudinal and Hall conductivities, σ_{yy} and σ_{xy} in the crossed field. Note that, for these classical expressions, σ_{xy} is proportional to B.

How does quantum mechanics revised this picture? For the classical model – **Drude theory**, the random elastic scattering of electrons impurities leads to a constant drift velocity in the presence of a constant electric field, $\sigma_0 = \frac{ne^2\tau}{m_e}$, where τ denotes the mean time between collisions. Now let us suppose the magnetic field is chosen so that number of electrons exactly fills all the Landau levels up to some N, i.e.

$$nL_xL_y = N\nu_{\max} \Rightarrow n = N\frac{eB}{h}\,.$$

The scattering of electrons must lead to a transfer between quantum states. However, if all states of the same energy are filled,[10] elastic (energy conserving) scattering becomes impossible. Moreover, since the next accessible Landau level energy is a distance $\hbar\omega$ away, at low enough temperatures, inelastic scattering becomes frozen out. As a result, the scattering time vanishes at special values of the field, i.e. $\sigma_{yy} \to 0$ and

$$\sigma_{\rm xy} \to \frac{ne}{B} = N\frac{e^2}{h}\,.$$

At critical values of the field, the Hall conductivity is quantized in units of e^2/h. Inverting the conductivity tensor, one obtains the resistivity tensor,

$$\left(\begin{array}{cc} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{array}\right) = \left(\begin{array}{cc} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{array}\right)^{-1},$$

where

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}, \qquad \rho_{xx} = -\frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2},$$

So, when $\sigma_{xx} = 0$ and $\sigma_{xy} = \nu e^2/h$, $\rho_{xx} = 0$ and $\rho_{xy} = h/\nu e^2$. The quantum Hall state describes dissipationless current flow in which the Hall conductance σ_{xy} is quantized in units of e^2/h. Experimental measurements of these values provides the best determination of fundamental ratio e^2/h, better than 1 part in 10^7.

[10]Note that electons are subject to Pauli's exclusion principle restricting the occupancy of each state to unity.