3. Quantum mechanics in a magnetic field

3.1. Charged particle in a magnetic field

$$\vec{F}_{Lorentz} = q\vec{E} + q\,\vec{v} \times \vec{B}$$

$$L(\vec{r}, \dot{\vec{r}}, t) = \frac{m}{2}\dot{\vec{r}}^2 - q\phi(\vec{r}) + q\,\dot{\vec{r}} \cdot \vec{A}(\vec{r})$$

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$$\vec{E} = -\nabla\phi - \dot{\vec{A}}$$

$$H(\vec{r}, \vec{p}, t) = \frac{1}{2m}\left(\vec{p} - q\,\vec{A}(\vec{r})\right)^2 + \underbrace{q\phi(\vec{r})}_{U(\vec{r})}$$

Canonical quantization:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{r}^2} + \frac{iq\hbar}{2m}\left(\frac{\partial}{\partial \vec{r}} \cdot \vec{A} + \vec{A} \cdot \frac{\partial}{\partial \vec{r}}\right) + \frac{q^2\vec{A}^2}{2m} + U(\vec{r})$$

Augment by spin and spin-orbit coupling (Pauli equation):

$$\hat{H}_{SB} = \frac{1}{2m^2c^2}\,\frac{1}{r}\,\frac{dU}{dr}\,\hat{\vec{L}} \cdot \hat{\vec{S}} - \gamma_S\,\vec{B} \cdot \hat{\vec{S}}$$

$$-\vec{S} \cdot (\vec{E} \times \vec{p})\,q$$

$$\vec{m} = \gamma\vec{L}$$

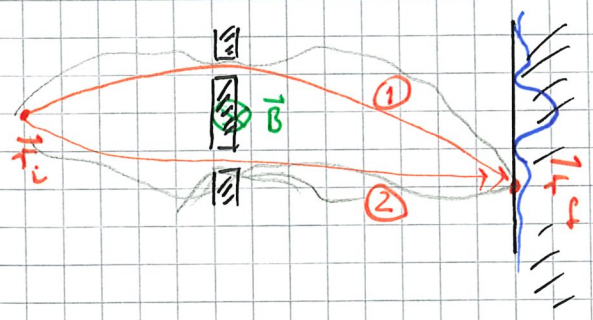
$$\gamma = \frac{q}{2m}g \qquad \left(\text{electron: } q<0,\ \gamma<0,\ g \hat{=} 2\right)$$

$$\left(\mu_B = \frac{\hbar|e|}{2m}\right)$$

In this chapter:

- Aharonov-Bohm effect
- Hydrogen atom + weak homog. field
- Free electrons + arbitrary homog. field

3.2. Aharonov - Bohm effect



Charged electrons, double slit.
Interference pattern depends on $\vec{B}$, although $\vec{B} = 0$ at all possible electron positions!

Consider

$$U(r_f, t_f; r_i, t_i) = \int_{r_i t_i}^{r_f t_f} \mathcal{D}[\vec{r}]\, e^{-i/\hbar\, S[\vec{r}]}$$

with

$$L = \underbrace{\frac{m}{2}\dot{\vec{r}}^2}_{L_0} + q\,\dot{\vec{r}}\cdot\vec{A}$$

$$S[\vec{r}] = S_0[\vec{r}] + q \underbrace{\int_{t_i}^{t_f} dt\, \dot{\vec{r}}\cdot\vec{A}}_{\int_{\vec{r}_i}^{\vec{r}_f} d\vec{r}\cdot\vec{A}}$$

Two different paths:



$$\int_{\vec{r}_1} d\vec{r}\cdot\vec{A} - \int_{\vec{r}_2} d\vec{r}\cdot\vec{A} = \oint d\vec{r}\cdot\vec{A} = \underbrace{\int d\vec{F}\cdot\vec{B}}_{\text{Flux } \Phi_F}$$

Split propagator into type-1 and type-2 paths, neglect loops:

$$U(r_f, t_f; r_i, t_i) = \left(\int_{(1)} + \int_{(2)} \right) \mathcal{D}[\vec{r}]\, e^{i/\hbar\, S[\vec{r}]}$$

$$\approx \exp\left(\frac{i}{\hbar} q \int_{(1)} d\vec{r}\cdot\vec{A}\right) \underbrace{\int_{(1)} \mathcal{D}[\vec{r}]\, e^{i/\hbar\, S_0[\vec{r}]}}_{P_1}$$

$$+ \exp\left(\frac{i}{\hbar} q \int_{(2)} d\vec{r}\cdot\vec{A}\right) \underbrace{\int_{(2)} \mathcal{D}[\vec{r}]\, e^{i/\hbar\, S_0[\vec{r}]}}_{P_2}$$

$$\boxed{\left|U(r_f, t_f; r_i, t_i)\right|^2 = \left|P_1 + e^{i\varphi} P_2\right|^2}$$

with

$$\varphi = \frac{q}{\hbar} \oint_{\text{"(1)-(2)"}} d\vec{r}\cdot\vec{A} = \frac{q}{\hbar}\Phi_F = 2\pi \frac{\Phi_F}{\Phi_0}$$

Interference pattern determined by flux (non-local!)

$\Phi_0 = \frac{h}{q}$ flux quantum

3.3. Reminder: Hydrogen atom

Non-relativistic, no fields.

$$\left(-\frac{\hbar^2}{2m}\Delta - \frac{e^2}{r} \right) \psi(\vec{r}) = E\,\psi(\vec{r})$$

Spectrum

$$E_n = -\frac{13.6\,\text{eV}}{n^2} = -\frac{1}{2n^2}\, e^4 \frac{m}{\hbar^2}$$

Principal quantum number: $n = \rho + \ell + 1$

Eigenfct $\psi_{n\ell m}(\vec{r}) = \underbrace{\frac{u_{n\ell}(r)}{r}}_{R_{n\ell}(r)} \cdot Y_{\ell m}(\theta, \varphi)$ ← spherical harmonics

with $R_{n\ell}(r) \propto e^{-r/na_0} \left(\frac{r}{na_0}\right)^{\ell} L^{2\ell+1}_{n-\ell-1}\left(\frac{2r}{na_0}\right)$

↖ Laguerre polynomials

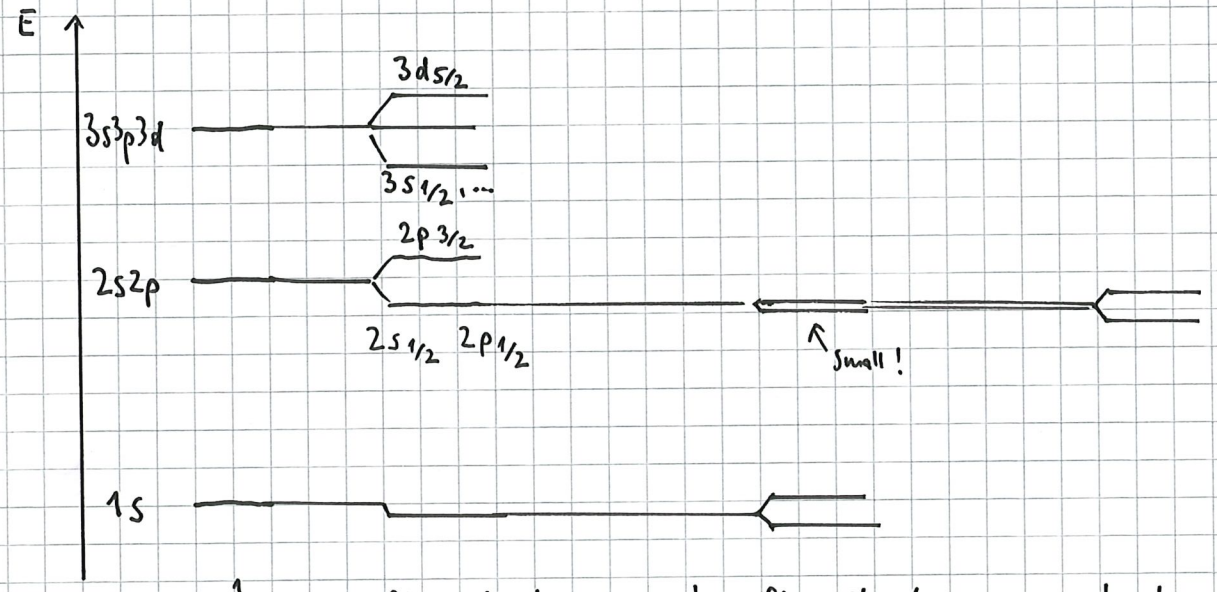
Bohr radius $a_0 = \frac{\hbar^2}{me^2} = 0.529\,\text{Å}$

m degeneracy from spherical symmetry $(m = -\ell, \dots, \ell)$

ℓ degeneracy from Runge-Lenz vector (specific to $1/r$ potential)

↖ $\vec{A} = \vec{p} \times \vec{L} - m\alpha\,\hat{e}_r$ for $V = \frac{\alpha}{r}$

Fine structure from spin-orbit coupling ↝ quantum number $j = \ell \pm \frac{1}{2}$



3.4. Hydrogen in weak magnetic field: Zeeman effect

Homogeneous field $\parallel z$: $\vec{B} = B\hat{e}_z$, $\vec{A} = \frac{1}{2}(\vec{B}\times\vec{r}) = \frac{B}{2}(\hat{e}_y x - \hat{e}_x y)$

$\operatorname{div}\vec{A} = 0 \rightsquigarrow \partial_{\vec{r}}\,\vec{A}\ldots = \vec{A}\,\partial_{\vec{r}}\ldots$

$\rightsquigarrow \frac{\partial}{\partial\vec{r}}\cdot\vec{A} + \vec{A}\cdot\frac{\partial}{\partial\vec{r}} = B\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = B\frac{i}{\hbar}\hat{l}_z$

Hence $\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3$

$\hat{H}_0 = -\frac{\hbar^2}{2m}\Delta + U(r)$

$\hat{H}_1 = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dU}{dr}\,\hat{\vec{l}}\cdot\hat{\vec{s}}$

$H_2 = -\frac{eB}{2m}\left(\hat{l}_z + 2\hat{s}_z\right) = -\frac{eB}{2m}\left(\hat{j}_z + \hat{s}_z\right)$ ($\uparrow g_{el}=2$)

$H_3 = \frac{e^2B^2}{8m}(x^2+y^2)$

Weak field $\hat{=}$ $\langle\hat{H}_2\rangle, \langle\hat{H}_3\rangle \ll \langle\hat{H}_0\rangle$ $<$ ⓐ $\langle\hat{H}_2\rangle \ll \langle\hat{H}_1\rangle$ ⓑ $\langle\hat{H}_0\rangle \gg \langle\hat{H}_2\rangle \gg \langle\hat{H}_1\rangle$

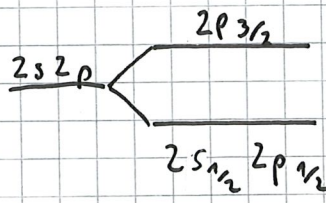
Zeeman effect: Shift of (atomic) level by (homogeneous) B field

(a) „Weak weak" field $\langle \hat{H}_2 \rangle \ll \langle \hat{H}_1 \rangle$

(field $\ll$ spin-orbit)

Unperturbed levels are fine-structure-split $|j\, m_j\, \ell\, s\rangle$

$(j = \ell \pm \frac{1}{2},\ -j \le m_j \le j)$



$$\langle j\, m_j\, \ell\, s \,|\, \hat{j}_z + \hat{s}_z \,|\, j\, m_j'\, \ell'\, s\rangle = \delta_{m_j m_j'}\delta_{\ell\ell'}\hbar m_j + \langle j m_j \ell s|\, \hat{s}_z\, |j m_j' \ell' s\rangle$$

Clebsch-Gordan: $|j m_j \ell s\rangle = \sum_{m_\ell m_s}' |\ell\, m_\ell\, s\, m_s\rangle\, C^{\ell m_j}_{\ell m_\ell s m_s}$

Explicitly $|\ell \pm \frac{1}{2}, m_j, \ell, s\rangle = \pm\,|\ell, m_j - \frac{1}{2}, s, \frac{1}{2}\rangle \sqrt{\frac{\ell \pm m_j + \frac{1}{2}}{2\ell+1}}$

$$+\,|\ell, m_j + \tfrac{1}{2}, s, -\tfrac{1}{2}\rangle \sqrt{\frac{\ell \mp m_j + \frac{1}{2}}{2\ell+1}}$$

Plug in to obtain

$$\langle j m_j \ell s \,|\, \hat{j}_z + \hat{s}_z \,|\, j m_j' \ell' s\rangle = \delta_{m_j m_j'}\delta_{\ell\ell'}\hbar m_j \left(1 \pm \frac{1}{2\ell+1}\right)$$

for $j = \ell \pm \frac{1}{2}$

$$\rightsquigarrow \quad \Delta E^{(1)}_{n\ell j m_j} = m_j\, \bar{g}\, \mu_B\, B \quad \text{with} \quad \bar{g} = 1 \pm \frac{1}{2\ell+1} \quad \text{for } j = \ell \pm \frac{1}{2}$$

$$\mu_B = \frac{\hbar |e|}{2m}$$

„Anomalous Zeeman effect"

(b) „strong" „weak" field $\langle \hat{H}_2 \rangle \gg \langle \hat{H}_1 \rangle$

(field $\gg$ spin-orbit)

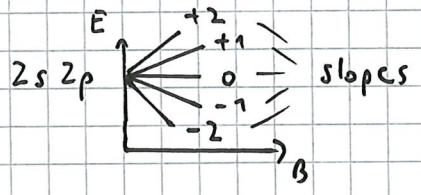
Neglect spin-orbit; unperturbed levels are $|\ell\, m_\ell\, s\, m_s\rangle$

$$\langle \ell\, m_\ell\, s\, m_s | \hat{\ell}_z + 2\hat{s}_z | \ell'\, m_\ell'\, s\, m_s' \rangle = \delta_{\ell\ell'}\,\delta_{m_\ell m_\ell'}\,\delta_{m_s m_s'}\,\hbar\,(m_\ell + 2m_s)$$

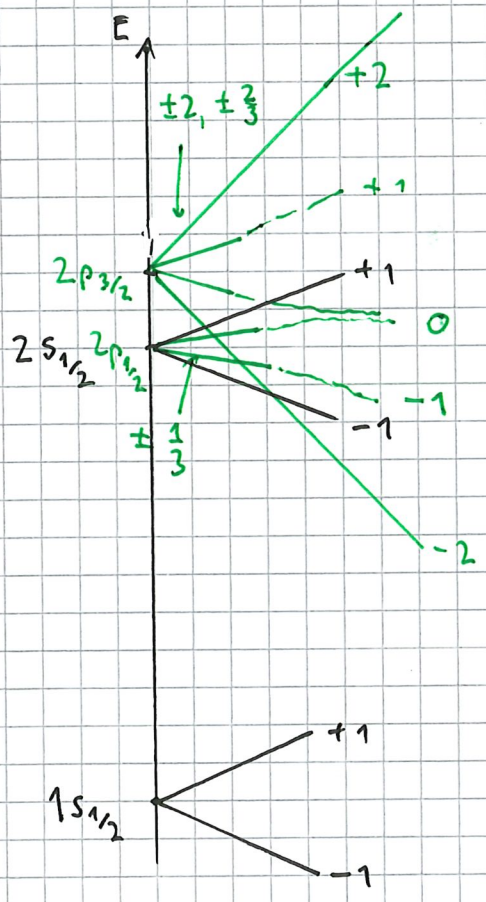
$$\curvearrowright \quad \Delta E^{(1)}_{n\, m_\ell\, m_s} = (m_\ell + 2m_s)\,\mu_B B$$

$-\ell, \ldots, \ell \qquad \pm\frac{1}{2}$

„Normal Zeeman effect"



Combine (a) & (b) (schematic, see Cohen-Tannoudji)



$$\bar{g}\,(2p_{3/2}) = \frac{4}{3}$$

$$\bar{g}\,(2p_{1/2}) = \frac{2}{3}$$

3.5. Free electrons in a magnetic field: Landau levels

Homogeneous magnetic field, represented by $\vec{A}$ ($\phi = 0$).

$$\hat{H} = \frac{1}{2m}\left(\vec{p} - e\vec{A}\right)^2 - \gamma\,\vec{B}\cdot\vec{s}$$

$\vec{B}$ homogeneous. Effect of spin trivial: split all levels by $\pm\frac{\hbar}{2}\gamma|\vec{B}|$

Now consider orbital motion only. Landau gauge $\vec{A} = (-By, 0, 0)$ for $\vec{B} = B\hat{e}_z$.

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_x + eB\hat{y}\right)^2 + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

Ansatz

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

Plug in:

$$\frac{1}{2m}\left[\hbar^2 k_x^2 + 2k_x eBy + (eB)^2 y^2\right]\chi - \frac{\hbar^2}{2m}\chi'' + \frac{\hbar^2 k_z^2}{2m}\chi = E\chi$$

$$-\frac{\hbar^2}{2m}\chi'' + \frac{m}{2}\omega_c^2 (y - y_0)^2\chi + \frac{\hbar^2 k_z^2}{2m}\chi = E\chi$$

with $\omega_c = \frac{|e|B}{m}$ (cyclotron frequency), $y_0 = -\frac{\hbar k_x}{eB}$

This describes harmonic oscillator (!) with frequency ω_c and equilibrium position y_0; last term is energy shift only.

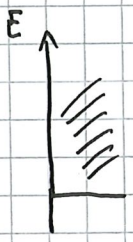
Eigenvalue spectrum

$$E(n, k_z) = \hbar\omega_c\left(n + \tfrac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m}$$

motion $\perp \vec{B}$ | motion $\parallel \vec{B}$

For fixed k_z the system has discrete energy levels (Landau levels), numbered by n, with spacing $\hbar\omega_c \propto |\vec{B}|$.

Energy spectrum (for k_z fix $\hat{=}$ 2-dim system)



$B = 0$

continuous spectrum



$\updownarrow \hbar\omega_c = \frac{\hbar |e| B}{m}$

$B > 0$

Landau levels (massively degenerate!)

Eigenstates of $\hat{H}$ (w/o proof):

$$\psi(x,y,z) \propto e^{ik_x x} e^{-\frac{1}{2}(y-y_0)^2/a_B^2} H_n\left(\frac{y-y_0}{a_B}\right) e^{ik_z z}$$

(with $y_0 = k_x a_B^2$, $a_B^2 = \frac{\hbar}{|e|B}$)

$\hat{=}$ plane wave $\parallel \hat{x}$ · oscillator along $\hat{y}$ · plane wave $\parallel \hat{z}$

Estimate of degeneracy (for finite system, in $d=2$):

degeneracy comes k_x (which determines y_0),

oscillator centre must be within system $\rightsquigarrow 0 < y_0 < L_y$

$$\rightsquigarrow 0 < k_x < \frac{|e|B}{\hbar} L_y$$

periodic boundary conditions along $\hat{x}$ $\rightsquigarrow$ quantized momenta $\Delta k_x = \frac{2\pi}{L_x}$

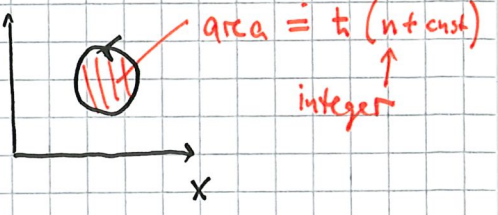
$\rightsquigarrow$ Number of states (for fixed n):

$$\frac{k_{x,\max}}{\Delta k_x} = \frac{|e|B}{\hbar} \frac{L_x L_y}{2\pi} = \Phi/\Phi_0 \qquad (\Phi_0 = \frac{hc}{|e|}$$ flux quantum)

Degeneracy scales with 2D system size!

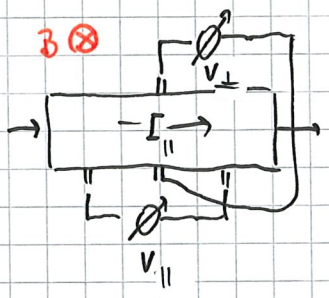
Semiclassical picture for Landau levels:

quantization of cyclotron orbits



3.6. Quantum Hall effect

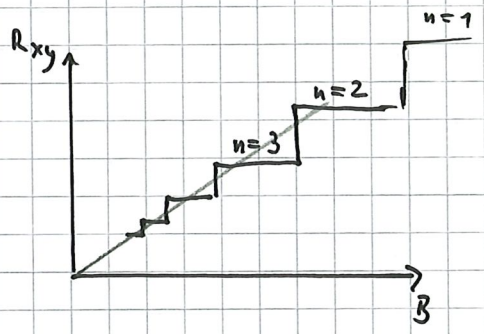
Electron gas in $d=2$ in magnetic field



Current generates transverse voltage from Lorentz force

Classical (Drude) $E_\perp = -v \cdot |B|$

$$\curvearrowright R_{xy} = \frac{V_\perp}{I_\parallel} = \frac{B}{n_{2d}\, e}$$



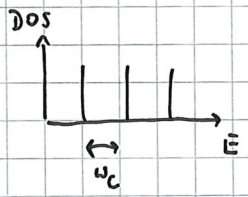
Observation: quantization

$$R_{xy} = \frac{1}{n}\,\frac{h}{e^2}$$

$$\left(\sigma_{xy} = n\,\frac{e^2}{h}\right)$$

Minimal explanation:

- Landau quantization



System is bulk insulator unless E_F coincides w/ Landau level (plateau transition)

- Hall current is carried by quantized edge states

Semiclassically: Skipping orbits



Each edge state contributes $\frac{e^2}{h}$ to σ_{xy}.

Experimentally, quantization is extremely precise (10^{-10}).