Landau orbits and their magnetic response

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Landau orbits

We consider the Hamiltonian of a charged particle in a constant magnetic field:

$$\mathcal{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - q_{\mathrm{e}}\vec{A}\right)^2$$

or more explicitly

$$\mathcal{H} = \frac{1}{2m}\left(\hat{p}^x + q_{\mathrm{e}}B\hat{y}\right)^2 + \frac{1}{2m}\left(\hat{p}^y - q_{\mathrm{e}}B\hat{x}\right)^2 + \frac{1}{2m}(\hat{p}^z)^2 \,.$$

with $\hat{p}^\alpha = -i\hbar\partial_\alpha$ being the linear momentum operator (quantum description). The $\hat{p}^z$ operator commutes with the Hamiltonian, therefore the wave function has the same dependence on z as the wave function of a free particle, and the same eigenvalues. The in-plane components can be rearranged to obtain the Hamiltonian of a harmonic oscillator, as it was first noted by Landau (1930). The resulting *Landau energy levels* read

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

where $n = 0, 1, 2...$ is an integer and $\omega_c = q_{\mathrm{e}}B/m$ the cyclotron frequency. For fixed n and k_z, neglecting the spin coordinate, the level degeneracy is

$$N_{\mathrm{d}} = L^2 q_{\mathrm{e}}B/(2\pi\hbar)$$

where L is the linear dimension of the system (see Ashcroft and Mermin *Solid-state Physics*).
We restrict ourselves to the case in which k_z is constant or, to make things simpler, to the 2D case setting $k_z = 0$.

Complete the passages to derive the partition function

$$\begin{aligned}\mathcal{Z} &= N_{\mathrm{d}}\sum_n \mathrm{e}^{-\beta E_n} \\ &= \dots \\ &= \dots \\ &= N_{\mathrm{d}}\frac{1}{2}\frac{1}{\sinh(\beta\hbar\omega_c/2)}\end{aligned}$$

Answer

$$
\begin{aligned}
\mathcal{Z} &= N_\mathrm{d} \sum_n \mathrm{e}^{-\beta E_n} \\
&= N_\mathrm{d} \mathrm{e}^{-\beta\hbar\omega_c/2} \sum_n \mathrm{e}^{-n\beta\hbar\omega_c} \\
&= N_\mathrm{d} \frac{\mathrm{e}^{-\beta\hbar\omega_c/2}}{1-\mathrm{e}^{-\beta\hbar\omega_c}} \\
&= N_\mathrm{d} \frac{1}{2} \frac{1}{\sinh(\beta\hbar\omega_c/2)}
\end{aligned}
$$

2. Using the partition function computed above, the average magnetic moment along z (direction along which the field is applied), can be computed

$$
\begin{aligned}
\langle \mu^z \rangle &= k_\mathrm{B} T \frac{1}{\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial B^z} \\
&= k_\mathrm{B} T \left[\frac{1}{B} - \frac{\beta q_\mathrm{e} \hbar}{2m} \coth(\beta\hbar\omega_c/2) \right] .
\end{aligned}
$$

(remember that N_d depends linearly on B!). By expanding the hyperbolic cotangent $\coth(x) = x^{-1} + x/3 + \mathcal{O}(x^5)$, compute the average magnetic moment $\langle \mu^z \rangle$ for small fields

For $\hbar\omega_c/(k_\mathrm{B}T) \ll 1$ one has

$$
\langle \mu^z \rangle = k_\mathrm{B} T \left[\frac{1}{B} - \frac{\beta q_\mathrm{e}\hbar}{2m} \left(\frac{2}{\beta\hbar\omega_c} + \frac{1}{3}\frac{\beta\hbar\omega_c}{2} + \ldots \right) \right] = -\frac{1}{12} \left(\frac{q_\mathrm{e}\hbar}{m} \right)^2 \frac{B}{k_\mathrm{B} T} .
$$

where the fact that $\omega_c = q_\mathrm{e}B/m$ and $\beta = 1/(k_\mathrm{B}T)$ was used.

3. What happens when $\hbar\omega_c/(k_\mathrm{B}T)$ goes to zero?

The classical result is recovered, namely a vanishing magnetic moment, in line with the Bohr–van Leeuwen theorem. This classical limit corresponds to the separation between energy levels becoming smaller than the thermal energy $k_\mathrm{B}T$.

Quiz Landau orbits *vs* single-electron atomic ordbitals

The average magnetic resulting from the quantization of the orbits of an electron that moves in a constant $\vec{B}$ field (Landau orbits) reads

$$
\langle \mu^z \rangle = k_\mathrm{B} T \left[\frac{1}{B} - \frac{\beta q_\mathrm{e}\hbar}{2m} \coth(\beta\hbar\omega_c/2) \right]
$$

and, as we have seen, it is negative (*diamagnetic*). The average magnetic moment of an *unpaired* electron occupying a single-electron atomic orbital (n, l, m) with $l \neq 0$ is instead positive (*paramagnetic*). This can be demonstrated computing its thermal average by means of the Zeeman single-electron Hamiltonian

$$
\mathcal{H}_{\mathrm{Z},i} = \mu_\mathrm{B}\, \hat{\mathbf{l}}_i \cdot \vec{B} \,.
$$

Indicate in the correct answer to the following questions with a X at the beginning of the corresponding line.

Question: Which main difference between the two sets of single-electron states is responsible for the opposite sign of $\langle \mu^z \rangle$ obtained in the two calculations?

- Landau orbits are eigenstates of a harmonic-oscillator Hamiltonian, while the (n, l, m) levels are eigenstates of a hydrogen-like Hamiltonian.
- In a semiclassical picture, Landau levels behave according to the Faraday-Neumann-Lenz law, while atomic $\langle \mu^z \rangle$ are the q.m. equivalent of Ampère's rigid, elementary current loops.
- **The origin of Landau orbits is the $\vec{B}$ field itself, while the (n, l, m) levels are eigenstates of the central-potential Hamiltonian $\mathcal{H}_{0,i}$ and can hardly be affected by the Zeeman interaction.**
- Both calculations produce $\langle \mu^z \rangle > 0$ for large enough B fields.