From Schrödinger to Dirac: Gauge Invariance, Landau Quantization, and Probability Currents

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I. GAUGE INVARIANCE

Using Maxwell equation [3]

$$\boldsymbol{\nabla} \cdot \vec{B} = 0, \tag{1}$$

$\vec{B}$ can be expressed as a the rotational of a vector potential $\vec{A}$:

$$\vec{B} = \nabla \times \vec{A}. \tag{2}$$

Therefore, by employing Faraday's law

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \Longrightarrow \nabla \times \big(\vec{E} + \frac{\partial \vec{A}}{\partial t}\big) = 0, \tag{3}$$

and therefore the last term, which has zero curl, can be expressed as the gradient of a scalar potential φ,

$$\vec{E} + \frac{\partial \vec{A}}{\partial t} = -\nabla\varphi \Longrightarrow \vec{E} = -\nabla\varphi - \frac{\partial \vec{A}}{\partial t}. \tag{4}$$

Thus we have $(\vec{E}, \vec{B})$ expressed in terms of the potentials $A \equiv (\varphi, \vec{A})$. We can also write the potentials as a four-vector $\{A^\mu\}$, where $\mu = 0, 1, 2, 3$, and $A^0 = \varphi$.

It is also noticeable that the potentials are not unique, two sets of potentials can give the same electromagnetic field. As a consequence of $\nabla \times (\nabla u) = 0$ (where u is any $\mathcal{C}_1$ function), the vector potential:

$$\vec{A}' = \vec{A} + \nabla\Lambda, \tag{5}$$

gives the same $\vec{B}$, but this changes $\vec{E}$, thus we have to transform φ accordingly:

$$\begin{aligned}\vec{E} &= -\nabla\varphi' - \frac{\partial \vec{A}'}{\partial t} \\ &= -\nabla\varphi' + \frac{\partial \vec{A}}{\partial t} - \frac{\partial(\nabla\Lambda)}{\partial t} \\ &= -\nabla(\varphi' + \frac{\partial \Lambda}{\partial t}) - \frac{\partial \vec{A}}{\partial t}.\end{aligned}$$

Hence, the transformation:

$$\begin{cases} \varphi' = \varphi - \dfrac{\partial \Lambda}{\partial t} \\ \vec{A}' = \vec{A} + \nabla\Lambda \end{cases} \tag{6}$$

leaves the electromagnetic fields unchanged, and therefore it is called a gauge transformation of the electromagnetic potential.

II. DYNAMICS OF A CHARGED PARTICLE IN AN EM FIELD

We will now show that, in classical mechanics, the dynamics of a particle with charge q, and mass m, can be described by the potential [2]

$$V = q\varphi - q\vec{A} \cdot \vec{v}, \tag{7}$$

or using relativistic notation

$$V = J^\mu A_\mu \tag{8}$$

where

$$J^\mu \equiv (q, q\vec{v}), \qquad A_\mu = \eta_{\mu\nu} A^\nu, \tag{9}$$

and we used the diagonal Minkowski metric $\eta_{\mu\mu} = [1, -1, -1, -1]$ This is indeed the potential if it leads, through the Euler-Lagrange equations, to the Lorentz force, and the Lagrangian is then given by

$$L = T - V = \frac{1}{2} m\vec{v}^2 - q\varphi + q\vec{A} \cdot \vec{v}. \tag{10}$$

For the x component, one gets

$$\frac{\partial L}{\partial x} = -q\frac{\partial \varphi}{\partial x} + q\frac{\partial \vec{A}}{\partial x} \cdot \vec{v}, \qquad \frac{\partial L}{\partial v_x} = mv_x + qA_x = p_x, \tag{11}$$

and thus the canonical momentum is no longer mv, instead it is

$$\vec{p} = m\vec{v} + q\vec{A}. \tag{12}$$

Now, deriving with respect to time the second equation in (11),

$$\frac{d}{dt}\frac{\partial L}{\partial v_x} = m\dot{v}_x + q\frac{dA_x}{dt} \tag{13}$$

applying the chain rule to the last term,

$$\frac{dA_x}{dt} = \frac{\partial A_x}{\partial t} + \sum_i \frac{\partial A_x}{\partial x_i} \cdot v_i, \tag{14}$$

and substituting in the Euler-Lagrange equation, one finally arrives at

$$\begin{aligned} m\dot{v}_x = -q\left(\frac{\partial \varphi}{\partial x} + \frac{\partial A_x}{\partial t}\right) + q\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)v_y + \\ +q\left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right)v_z = qE_x + q(B_z v_y - B_y v_z) = \\ = q(\vec{E} + \vec{v} \times \vec{B})\Big|_x. \end{aligned}$$

And equivalently for the y and z components, we obtain the Lorentz force, as expected.

Therefore, the potential stated in Eq. (7) is correct, so we can proceed to obtain the Hamiltonian through a Legendre transformation

$$H = \sum_i p_i \cdot \dot{q}_i - L = \sum_i \frac{1}{2} m v_i^2 + q\varphi, \tag{15}$$

which after substitution from (12), leads to the Hamiltonian as a function of $\vec{p}$ and $\vec{x}$:

$$H = \frac{1}{2m}\left(\vec{p} - q\vec{A}\right)^2 + q\varphi. \tag{16}$$

For quantum mechanics we only have to substitute the quantities $\vec{p}$ and $\vec{x}$ by their quantum operators:

$$\begin{cases} \vec{p} \longrightarrow \hat{p}, \\ \vec{x} \longrightarrow \hat{x}, \end{cases} \tag{17}$$

which satisfy the commutation relation $[\hat{x}, \hat{p}] = i\hbar$, and $\vec{A}$ and φ also become operators, as functions of the position $\hat{x}$ and time. Thus the quantum Hamiltonian operator can be written as

$$\hat{H} = \frac{1}{2m}\left(\hat{p} - q\hat{A}\right)^2 + q\hat{\varphi}. \tag{18}$$

III. SCHRÖDINGER EQUATION

The Schrödinger equation is given by [6]

$$i\hbar\frac{\partial \Psi}{\partial t} = \hat{H}\Psi, \tag{19}$$

so we only have to substitute in it the Hamiltonian that we have just obtained, but we now that the canonical momentum $\hat{p}$ acts like $\frac{\hbar}{i}\nabla$ in position space, thus

$$i\hbar\frac{\partial \Psi}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)^2 + q\varphi\right]\Psi. \tag{20}$$

But as we saw in Section I, the potentials were not unique, and we could use another pair $(\varphi', \vec{A}')$ that returns the same fields $(\vec{E}, \vec{B})$. So we ask ourselves if by using

$$i\hbar\frac{\partial \Psi'}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}'\right)^2 + q\varphi'\right]\Psi', \tag{21}$$

we can get the same wave-function $\Psi' \stackrel{?}{=} \Psi$. The answer is no, since we get a shift in phase, but we still obtain the same probabilities, and expectation values, as the phase gets erased when the wave-function is squared. Now, we will see that the wave-function transforms accordingly as

$$\Psi' = \Psi e^{i\frac{q}{\hbar}\Lambda(x,t)}, \tag{22}$$

when the potentials transform as written in (6). It is important to notice that this transformation depends on the position and time through the arbitrary function Λ.

IV. GAUGE INVARIANCE OF THE SCHRÖDINGER EQUATION

We will denote by U the unitary transformation $e^{i\frac{q}{\hbar}\Lambda(x,t)}$, hence $\Psi' = U\Psi$. Then, by expanding the Hamiltonian (18) [6]

$$\hat{H} = \frac{1}{2m}\left[\vec{p}^2 - q\vec{p}\cdot\vec{A} - q\vec{A}\cdot\vec{p} + (q\vec{A})^2\right], \tag{23}$$

and since $\vec{p}$ and $\vec{A}$ do not commute, by acting with $\vec{p}\cdot\vec{A}$ on a generic wave function Ψ, one obtains

$$\vec{p}\cdot(\vec{A}\Psi) = \frac{\hbar}{i}(\boldsymbol{\nabla}\cdot A)\Psi + \vec{A}\cdot\vec{p}\Psi. \tag{24}$$

With this result, the Hamiltonian can be rewritten as

$$\hat{H} = \frac{1}{2m}\left[\vec{p}^2 - q\frac{\hbar}{i}(\boldsymbol{\nabla}\cdot A) - 2q\vec{A}\cdot\vec{p} + (q\vec{A})^2\right]. \tag{25}$$

Now, we are going to study the covariant derivative $\hat{\Pi} = (\hbar/i)\nabla - q\vec{A}$:

$$\begin{aligned}\left(\frac{\hbar}{i}\nabla - q\vec{A}'\right)\Psi' &= \left(\frac{\hbar}{i}\nabla - q\vec{A}'\right)U\Psi = \\ = \frac{\hbar}{i}(\nabla U)\Psi + U\frac{\hbar}{i}\nabla\Psi &- q\vec{A}U\Psi - q(\nabla\Lambda)U\Psi = \\ &= U\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)\Psi.\end{aligned}$$

As can be seen, if we transform both the potential and the wave-function, this derivative remains the same, and this is the one that appears squared in the Hamiltonian (18). Then, we only have to see if the rest of Eq. (20), $i\hbar\partial_t - q\varphi$ is also covariant, where we have moved the $q\varphi$ term to the other side of the equation, that is

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t} - q\varphi'\right)\Psi' &= \left(i\hbar\frac{\partial}{\partial t} - q\left(\varphi - \frac{\partial\Lambda}{\partial t}\right)\right)U\Psi = \\ &= U\left(i\hbar\frac{\partial}{\partial t} - q\varphi\right)\Psi.\end{aligned}$$

One concludes that if both the potentials and the wave-function are transformed, Eq. (21) implies (20), and hence the Schrödinger equation is gauge invariant. Since the phase change does not alter probabilities nor expectation values, the resulting physics remains the same.

V. APPLICATION: LANDAU LEVELS

Imagine we have a particle with charge q and mass m confined in a plane (we ignore the z direction), and a constant magnetic field $\vec{B} = B\hat{z}$ is applied along the z axis [6]. We can describe this field with the vector potential $\vec{A} = (0, Bx, 0)$, because by applying (2) we recover our magnetic field. Therefore the Hamiltonian, using Eq (25), reads

$$\hat{H} = \frac{1}{2m}\left[p_x^2 + p_y^2 - 2qBxp_y + (qBx)^2\right]. \tag{26}$$

But, as p_y commutes with the Hamiltonian, $[p_y, H] = 0$, because there is no y dependence in $\hat{H}$, the eigenfunctions can be written as $\Psi = \psi(x)e^{ik_y y}$, which gives

$$\hat{H}\Psi = \frac{1}{2m}\left[(\hbar k_y)^2 + p_x^2 - 2qBx\hbar k_y + (qBx)^2\right]\Psi = \\ = \frac{1}{2m}\left[p_x^2 + (qBx - \hbar k_y)^2\right]\Psi = \\ = \left[\frac{p_x^2}{2m} + \frac{1}{2}m\left(\frac{qB}{m}\right)^2\left(x - \frac{\hbar k_y}{qB}\right)^2\right]\Psi$$

After renaming $\omega_B = qB/m$ and $x_0 = \hbar k_y/(qB)$, a harmonic oscillator in the x direction results. Therefore it has solutions $|n_x\rangle$ with energies $E(n_x, k_y) = \hbar\omega_B(n_x + \frac{1}{2}) = E_{n_x}$ that do not depend on k_y. These are the Landau levels. The characteristic length scale is the oscillator

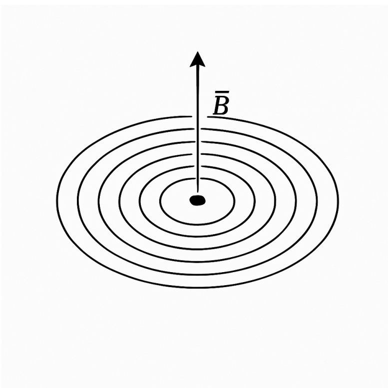

FIG. 1. Landau levels (Classical orbits)

length

$$d = \sqrt{\frac{\hbar}{m\omega_B}} = \sqrt{\frac{\hbar}{qB}} \equiv l_B, \tag{27}$$

where we have defined the magnetic length l_B, so we can rewrite $x_0 = k_y l_B^2$

By using other gauges, we would have obtained the same energies with different eigenfunctions, but they have to comprehend the same eigenspace, which has a high energy degeneracy (there is an infinite degeneracy in k_y for an infinite system). For example, with the potential $\vec{A} = (-By, 0, 0)$, we would have obtained eigenfunctions with plane waves along the x direction. Or else, we could have used a more symmetric gauge $\vec{A} = B/2(-y, x, 0)$, which reproduces the classical circular orbits, with the same frequency ω_B, but they are now quantized.

VI. LANDAU LEVELS: FINITE SAMPLE

In the last section we considered that the particle was confined in an infinite plane, now we will study a 2D, finite system with lengths L_x and L_y along directions x and y, respectively, with sides starting at the origin of coordinates [6]. In addition, we impose periodic boundary conditions along the y direction, so that

$$e^{ik_y y} = e^{ik_y(y+L_y)} \Longrightarrow k_y = \frac{2\pi n_y}{L_y}. \tag{28}$$

Then n_y is restricted to be $\bar{n}_y > n_y > 0$, because k_y has to be positive in order for x_0 to be positive. and there is a maximum value $\bar{n}_y$ because there is also one for x_0 when $x_0 = L_x$, that is

$$\bar{n}_y = \left\lfloor \frac{L_x L_y}{2\pi l_B^2} \right\rfloor, \tag{29}$$

where $\lfloor x \rfloor$ indicates the integer part of x. This $\bar{n}_y$ is in fact the number of states with the same energy (so identical Landau level) that fit our finite sample. And therefore it is also the degeneracy of the Landau levels, which is the same for them all (it does not depend on n_x).

This degeneracy, in terms of the area $A = L_x L_y$, and then of the magnetic flux, reads

$$\bar{n}_y \equiv D = \left\lfloor \frac{AB}{2\pi\hbar/q} \right\rfloor = \left\lfloor \frac{\Phi}{\Phi_0} \right\rfloor, \tag{30}$$

where $\Phi_0 = 2\pi\hbar/q$, with q being the absolute value of the electron charge, is called the flux quantum.

VII. PROBABILITY CURRENT OF THE LANDAU LEVELS

The probability current density in quantum mechanics is given by [1]:

$$\vec{J}(\vec{r}, t) = \frac{1}{2m}\left[\psi^*\left(\tfrac{\hbar}{i}\nabla - q\vec{A}\right)\psi + \text{c.c.}\right] \\ = \frac{1}{m}\,\text{Re}\{\psi^*(\hat{\vec{p}} - q\vec{A})\psi\}, \tag{31}$$

and it enters the continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot\vec{J} = 0, \tag{32}$$

where $\rho = |\Psi|^2$, which states the conservation of probability $\int \rho\, dx = 1$.

The continuity equation can also be rewritten, more compactly, in relativistic notation

$$\partial_\mu J^\mu = 0 \tag{33}$$

as a conserved current, where $J^\mu \equiv (\rho, \vec{J})$

Now we will substitute in these expressions the eigenstates of the Hamiltonian that we have obtained previously.

A. Eigenstates in the Landau Gauge

The normalized eigenfunctions can be written as

$$\begin{aligned}\Psi_{n_x,k_y}(x,y,t) &= e^{-iE_{n_x}t/\hbar}\,\psi(x,y),\\ \psi(x,y) &= e^{ik_y y}\,\varphi_{n_x}\left(x-x_0\right),\end{aligned} \tag{34}$$

where $x_0 = \hbar k_y/(qB)$, and

$$\varphi_n(u) = \frac{1}{\sqrt{l_B 2^n n! \sqrt{\pi}}}\,e^{-u^2/2}\,H_n(u). \tag{35}$$

are the harmonic oscillator eigenfunctions [1], and $u = (x-x_0)/l_B$, although, for the sake of simplifying the notation, we will be writing $\varphi_{n_x}(u) \equiv \varphi_{n_x}(x-x_0)$ or just φ_{n_x} with the implicit argument and length scale $l_B = \sqrt{\hbar/m\omega_B}$.

B. Current Density for a Single Landau State

By using

$$\begin{aligned}-q\vec{A}\,\psi &= (0, -qB\,x\,, 0)\,\psi,\\ \nabla\psi &= e^{ik_y y}\big(\partial_x\varphi_{n_x},\ ik_y\varphi_{n_x},\ 0\big),\end{aligned} \tag{36}$$

we obtain

$$\vec{J}_{n_x,k_y}(x,y) = \frac{\varphi_{n_x}^2}{m}\,(0,\ \hbar k_y - qBx,\ 0). \tag{37}$$

This shows that the probability current flows in the y-direction with a local velocity proportional to $(\hbar k_y - qBx)/m$, and that its divergence vanishes, therefore, from the continuity equation (32), $\partial_t\rho = 0$.

C. Superposition of eigenfunctions in the same Landau Level

Let the wavefunction be a generic superposition of eigenfunctions, with equal n_x and therefore with equal energy, that we have found with our gauge

$$\Psi_{n_x}(x,y,t) = e^{-iE_n t/\hbar}\sum_{k_y} c_{k_y}\,e^{ik_y y}\,\varphi_{n_x}^{(k_y)}, \tag{38}$$

where $\sum_{k_y}|c_{k_y}|^2 = 1$. Although by replacing the sums with integrals we could have obtained the alternative solutions derived with different gauges, the discrete approach is valid to show that these states preent a stationary probability current. The interference between different k_y components yields cross terms $\Psi_{n_x}^*(\hbar/i\nabla - q\vec{A})\Psi_{n_x}$, that lead to current densities $\vec{J}(x,y) = (J_x, J_y, 0)$ with

$$\begin{aligned}J_x &= \mathrm{Re}\left\{\frac{\hbar}{i\,m}\sum_{k_y,k_y'} c_{k_y}c_{k_y'}\,e^{i(k_y-k_y')y}\varphi_{n_x}^{(k_y')}\partial_x\varphi_{n_x}^{(k_y)}\right\},\\ J_y &= \mathrm{Re}\left\{\sum_{k_y,k_y'} c_{k_y}c_{k_y'}^*\,e^{i(k_y-k_y')y}\,\frac{\hbar k_y - qBx}{m}\varphi_{n_x}^{(k_y)}\varphi_{n_x}^{(k_y')}\right\}.\end{aligned} \tag{39}$$

This expression contains interference terms with wave numbers $k_y - k_y'$. The case with only one non-zero coefficient $c_{k_y} = \delta_{k_y q}$ retrieves the result from the former section.

D. Stationarity Probability Current

All Landau modes share the same energy E_{n_x}, so the probability density is time independent

$$\rho(x,y) = \sum_{k_y,k_y'} c_{k_y}c_{k_y'}^*\,e^{i(k_y-k_y')y}\varphi_n^{(k_y)}\varphi_n^{(k_y')}, \tag{40}$$

so $\partial_t\rho = 0$, and by the continuity equation $\boldsymbol{\nabla}\cdot\vec{J} = 0$.

It could also be shown computing the divergence of $\vec{J}$ directly, and this result implies that all eigenstates of the hamiltonian with an energy E_{n_x} (for every gauge), has a stationary current, which makes sense since they are eigenstates of $\hat{H}$ and thus stationary states, which means they do not have time dependence.

VIII. PAULI EQUATION

If we introduce the spin degree of freedom for a spin-1/2 particle, the Schrödinger equation

$$\hat{H}\,\chi = i\hbar\,\partial_t\chi, \tag{41}$$

becomes a matrix equation for the two-component Pauli spinor

$$\chi = \begin{pmatrix}\chi_\uparrow\\ \chi_\downarrow\end{pmatrix}. \tag{42}$$

Intuitively, $\hat{H}$ must be a 2×2 operator acting on a two-component column vector. In the absence of electromagnetic fields the momentum operator is justt $\hat{p} = -i\hbar\nabla$, and one may write the matrix version of the free Hamiltonian for the scalar system as

$$\hat{H} = \frac{1}{2m}(\vec{\sigma}\cdot\hat{p})(\vec{\sigma}\cdot\hat{p}), \tag{43}$$

by using the Pauli identity [6]

$$(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = (\vec{a}\cdot\vec{b})\,\mathbb{1} + i\,\vec{\sigma}\cdot(\vec{a}\times\vec{b}), \tag{44}$$

and the fact that $\vec{p}\times\vec{p} = 0$,, Eq. (43) is just $\hat{H} = \hat{p}^2/(2m)\,\mathbb{1}$.

In the presence of electromagnetic potentials we replace $\hat{p}$ by $\vec{\pi} = \hat{p} - q\,\vec{A}$, and $\hat{H}$ by $\hat{H} - q\hat{\varphi}$ to obtain

$$\hat{H} = \frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\vec{\pi}) + q\,\hat{\varphi}. \tag{45}$$

Notice that $[\pi_i, \pi_j] \neq 0$, since the $\vec{p}$ and $\vec{A}$ vector operators do not commute, therefore one finds [6]

$$\vec{\pi}\times\vec{\pi} = i\hbar\,q\,\vec{B}, \tag{46}$$

so that the expanded Pauli Hamiltonian Eq. (45) reads

$$\hat{H}_{\text{Pauli}} = \frac{(\hat{p} - q\vec{A})^2}{2m} - \frac{q\hbar}{2m}\,\vec{\sigma}\cdot\vec{B} + q\,\hat{\varphi}. \tag{47}$$

Finally, by using the relationship between magnetic dipole moment $\vec{\mu}$ and angular momentum, $\vec{\mu} = g\,q/(2m)\vec{S}$, in this case the (intrinsic) spin angular momentum of the particle $\vec{S} = (\hbar/2)\vec{\sigma}$ with g-factor $g = 2$, the previous equation can be rewritten as

$$\hat{H}_{\text{Pauli}} = \frac{(\hat{p} - q\vec{A})^2}{2m} - \vec{\mu}\cdot\vec{B} + q\,\hat{\varphi}, \tag{48}$$

showing explicitly the interaction energy of a magnetic dipole in an external magnetic field.

We will now use this equation to study the Landau levels but for a spin-1/2 particle, in the non-relativistic limit.

IX. LANDAU LEVELS FOR A SPIN 1/2 PARTICLE

Since $\varphi = 0$ and $\vec{B} = (0, 0, B)$, the Pauli Hamiltonian reduces to:

$$\hat{H} = \frac{(\hat{p} - q\vec{A})^2}{2m} - \frac{q\hbar B}{2m}\,\sigma_z = \frac{(\hat{p} - q\vec{A})^2}{2m} - \omega_B\,\hat{S}_z. \tag{49}$$

The first term is the *orbital* Hamiltonian $\hat{H}_{\text{orb}}$ (identical to the scalar Landau problem we solved in V), and the second term defines the *spin* Hamiltonian $\hat{H}_{\text{spin}} = -\omega_B\hat{S}_z$. Therefore, the total Hamiltonian splits as $\hat{H} = \hat{H}_{\text{orb}} + \hat{H}_{\text{spin}}$ (it is separable), so the eigenstates are tensor products $|n_x, k_y, \varepsilon\rangle = |n_x, k_y\rangle \otimes |\varepsilon\rangle$, where $\varepsilon = \uparrow, \downarrow$ indicates the eigenstates of $\hat{H}_{\text{spin}}$,

$$-\omega_B\hat{S}_z\,|\uparrow\rangle = -\frac{\hbar\omega_B}{2}\,|\uparrow\rangle, \tag{50}$$

$$-\omega_B\hat{S}_z\,|\downarrow\rangle = \frac{\hbar\omega_B}{2}\,|\downarrow\rangle. \tag{51}$$

that shift each Landau level up or down in energy by the amount $\mp\hbar\omega_B/2$ (see Fig. 2).

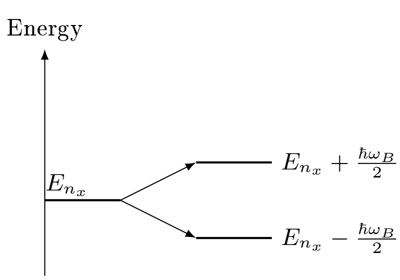

FIG. 2. Splitting of the nth Landau level by the Pauli term $-\omega_B S_z$.

Putting both contributions together, the total energy eigenvalues are

$$E_{n_x,\varepsilon} = \hbar\omega_B\left(n_x + \tfrac{1}{2}\right) \mp \frac{\hbar\omega_B}{2}. \tag{52}$$

Notice that this shift is the same for all landau levels, since it does not depend on the orbital quantum number n_x, and it also coincides with the energy difference between Landau levels $\hbar\omega_B$, so in this new system with spin, we have a fundamental level that is alone, and all other levels that go in pairs, for example, $|0, k_y, -\rangle$ has the same energy that $|1, k_y, +\rangle$, thus we could observe a current between these two levels as the energy is conserved, which means a current between two different spin states, a phenomena we will discuss later in section XIV.

X. PROBABILITY CURRENT FOR A SPIN-1/2 PARTICLE

A. Probability current expression

The probability density of the spin-1/2 particle is $\rho = \chi^\dagger\chi$, where $\chi^\dagger = [\chi_\uparrow^*\,\chi_\downarrow^*]$ is a row vector, and its time derivative gives

$$\partial_t\rho = \chi^\dagger\,\partial_t\chi + (\partial_t\chi^\dagger)\,\chi \tag{53}$$

$$= \frac{1}{i\hbar}\Big[\chi^\dagger\hat{H}\chi - (\chi\hat{H}\chi^\dagger)\Big], \tag{54}$$

where, in the second row, we used the Pauli equation (41) and its complex conjugate equation, and the fact that $\hat{H}$ is Hermitian. Next, we substitute $\hat{H} = (\vec{p}^{\,2}/2m) - \omega_B\hat{S}_z$ to get

$$\chi^\dagger\,\partial_t\chi + (\partial_t\chi^\dagger\,\chi) = \frac{1}{i\hbar}\Big[\chi^\dagger\tfrac{\vec{p}^{\,2}}{2m}\chi - \text{c.c.}\Big]. \tag{55}$$

because the spin term cancels. Finally, we use the equality $\frac{1}{i\hbar}\left(\chi^\dagger\vec{p}^{\,2}\chi - \text{c.c.}\right) = \nabla[\chi^\dagger\vec{p}\chi + \text{c.c.}]$, to recover the same current density as for the spinless particle (31):

$$\frac{\partial\rho}{\partial t} + \nabla\vec{J} = 0, \tag{56}$$

where the probability current density is $\vec{J} = \text{Re}\left[\chi^\dagger\vec{p}\chi\right]/m$.

B. Substitution on Landau Eigenstates

For the Landau-level eigenstates $|n, k_y, \uparrow\rangle$,with spin components $\chi = (\chi_\uparrow, 0)^T$ and $\chi_\uparrow = |n, k_y\rangle$, the current density reads

$$\vec{J} = \frac{1}{m}\,\text{Re}\{\chi^\dagger[\tfrac{\hbar}{i}\nabla - q\vec{A}]\chi\}, \tag{57}$$

where $\nabla\chi = (\nabla\chi_\uparrow, 0)^T$ and $q\vec{A}\chi = qB\,x\,\hat{y}\,\chi$, so that $[\hbar/i\nabla - q\vec{A}]\chi$, matches formally the equivalent expressions for the scalar case (see Section VII B), and the probability current for the spin-1/2 Landau problem is the same as in the spinless problem.

C. Superposition of Spin Components

We now consider a generic two-component spinor of the type

$$\chi = \begin{pmatrix} \chi_\uparrow \\ \chi_\downarrow \end{pmatrix} = \begin{pmatrix} c_1 \, |n_x, k_y\rangle \\ c_2 \, |n_x', k_y'\rangle \end{pmatrix},$$

with the normalization condition $|c_1|^2 + |c_2|^2 = 1$. Since there are no cross-terms in the current, each component contributes independently, and

$$\vec{J} = |c_1|^2 \, \vec{J}_\uparrow \; + \; |c_2|^2 \, \vec{J}_\downarrow, \tag{58}$$

where, exactly as in the scalar Landau problem,

$$\vec{J}_\uparrow = \frac{\varphi_{n_x}^2\big(x - x_0(k_y)\big)}{m} \big(0, \; \hbar k_y - qBx, \; 0\big), \tag{59}$$

$$\vec{J}_\downarrow = \frac{\varphi_{n_x'}^2\big(x - x_0(k_y')\big)}{m} \big(0, \; \hbar k_y' - qBx, \; 0\big). \tag{60}$$

Therefore, the currents simply add linearly, whith the factor c_i squared, which makes sense as we are dealing with probabilities. If instead we take a superposition over different k_y for each spin component, we recover again the same interference-current structure derived in Section VII C for each spinor component. Also, $\boldsymbol{\nabla} \cdot J = 0$ as expected for stationary states. ¡¡

XI. DIRAC EQUATION

In relativity the energy–momentum relation is [6]

$$E^2 = (c\,\vec{p})^2 + (mc^2)^2. \tag{61}$$

We seek a linear operator equation of the form $(c\,\vec{\alpha} \cdot \hat{p} + \beta mc^2)^2 = (c\,\hat{p})^2 + (mc^2)^2$, where $\vec{\alpha} \cdot \hat{p} = \alpha_1 p_x + \alpha_2 p_y + \alpha_3 p_z$, and the matrices must satisfy

$$\alpha_i^2 = \beta^2 = \hat{\mathbb{1}}, \qquad \text{(4 constraints)}, \tag{62}$$

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 0 \quad (i \neq j), \qquad \text{(3 constraints)}, \tag{63}$$

$$\alpha_i \beta + \beta \alpha_i = 0, \qquad \text{(3 constraints)}. \tag{64}$$

In total there are 10 algebraic restrictions (plus Hermiticity) on the matrices α_i, β.

EXPLICIT CONSTRUCTION OF THE DIRAC MATRICES

It turns out that the algebraic constraints require at least 4×4 matrices. One convenient representation is [6]:

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \hat{\mathbb{1}}_{2\times2} & 0 \\ 0 & -\hat{\mathbb{1}}_{2\times2} \end{pmatrix}, \tag{65}$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices and $\hat{\mathbb{1}}_{2\times2}$ is the 2×2 identity.

One checks directly:

$$\beta^2 = \begin{pmatrix} \hat{\mathbb{1}} & 0 \\ 0 & -\hat{\mathbb{1}} \end{pmatrix}^2 = \hat{\mathbb{1}}_{4\times4}, \tag{66}$$

$$\{\alpha_i, \alpha_j\} = \alpha_i \alpha_j + \alpha_j \alpha_i = 2\,\delta_{ij}\,\hat{\mathbb{1}}_{4\times4}, \tag{67}$$

$$\{\alpha_i, \beta\} = \alpha_i \beta + \beta \alpha_i = 0. \tag{68}$$

Thus $\vec{\alpha}$ and β satisfy all required anti-commutation and squaring relations.

We still have free parameters, so the pair $(\vec{\alpha}, \beta)$ is not unique.

Finally, the Dirac Hamiltonian takes the compact form

$$\hat{H}_{\text{Dirac}} = c\,\vec{\alpha} \cdot \hat{p} + \beta\, mc^2. \tag{69}$$

The Dirac equation in the presence of electromagnetic fields with usual change $\hat{p} \rightarrow \hat{\pi} = \hat{p} - q\vec{A}$:

$$i\hbar\,\partial_t \Psi = \hat{H}_{\text{Dirac}}\,\Psi, \quad \Psi = \begin{pmatrix} \chi \\ \phi \end{pmatrix}, \qquad \hat{H}_{\text{Dirac}} = c\,\vec{\alpha} \cdot \vec{\pi} + \beta\, mc^2 + q\,\varphi. \tag{70}$$

Where χ and ϕ are Pauli spinors, so the wave-function has four components.

XII. PAULI EQUATION FROM THE DIRAC EQUATION

We now intend to derive the Pauli equation as a non-relativistic limit of the Dirac equation.

In component form one obtains

$$i\hbar\,\partial_t \chi = c\,\vec{\sigma} \cdot \vec{p}\,\phi + mc^2\,\chi, \tag{71}$$

$$i\hbar\,\partial_t \phi = c\,\vec{\sigma} \cdot \vec{p}\,\chi - mc^2\,\phi. \tag{72}$$

Assuming energies near the rest mass, set $E = \mathcal{E} + mc^2$ with $\mathcal{E} \ll mc^2$, and solve for the "small" component:

$$\phi \approx \frac{c\,\vec{\sigma} \cdot \vec{p}}{E + mc^2}\,\chi \approx \frac{\vec{\sigma} \cdot \vec{p}}{2mc}\,\chi. \tag{73}$$

$(pc \ll mc^2)$, in the non-relativistic limit, which implies $(\phi \ll \chi)$ Substituting back into the upper-component equation (71) yields

$$\mathcal{E}\,\chi = \frac{(\vec{\sigma} \cdot \vec{p})^2}{2m}\,\chi, \tag{74}$$

which is the Pauli Hamiltonian (we ignore the second equation (72), since ϕ is small), so we conclude it is indeed the non-relativistic limit of the Dirac Hamiltonian.

XIII. PROBABILITY CURRENT FOR THE DIRAC EQUATION

As in non-relativistic quantum mechanics, the probability density $\rho = \Psi^\dagger \Psi = |\Psi|^2$, so that

$$\partial_t \rho = \partial_t(\Psi^\dagger \Psi) = (\partial_t \Psi^\dagger)\Psi + \Psi^\dagger(\partial_t \Psi). \tag{75}$$

From the Dirac Hamiltonian $i\hbar\,\partial_t\Psi = [\,c\,\vec{\alpha}\cdot\vec{p}+\beta\,mc^2]\,\Psi$ we have

$$\partial_t\Psi = -\tfrac{i}{\hbar}[\,c\,\vec{\alpha}\cdot\vec{p}+\beta\,mc^2]\,\Psi, \quad (76)$$

$$\partial_t\Psi^\dagger = +\tfrac{i}{\hbar}\Psi^\dagger[\,c\,(\vec{\alpha}\cdot\vec{p})^\dagger+\beta\,mc^2]. \quad (77)$$

Since $(\vec{\alpha}\cdot\hat{p})^\dagger = \vec{\alpha}\cdot\hat{p}$ (the α^i are Hermitian) and $\beta^\dagger = \beta$, substitution gives

$$\partial_t\rho = -\tfrac{i}{\hbar}\big[\Psi^\dagger(c\,\vec{\alpha}\cdot\hat{p})\Psi - (c\,\vec{\alpha}\cdot\hat{p}\Psi)^\dagger\Psi\big]. \quad (78)$$

Using $\hat{p} = -i\hbar\nabla$ and $(\hat{p}\Psi)^\dagger = +i\hbar\nabla\Psi^\dagger$, which implies $\nabla^\dagger \equiv -\nabla$, one shows $\partial_t\rho + \nabla\cdot\vec{J} = 0$ with

$$\vec{J} = c\,\Psi^\dagger\vec{\alpha}\,\Psi. \quad (79)$$

Thus the Dirac probability current is $J^0 = \Psi^\dagger\Psi$, $\vec{J} = c\,\Psi^\dagger\vec{\alpha}\Psi$. This is shown easily in relativistic notation, and defining

$$\gamma = (\beta, \gamma^0\vec{\alpha}) \quad (80)$$

We arrive at the continuity equation (33) with $J^\mu = \bar{\Psi}\gamma^\mu\Psi$, with the adjunct spinor $\bar{\Psi} = \Psi^\dagger\gamma^0$ (see [5]).

XIV. PAULI CURRENT AS A LIMIT FROM DIRAC

Starting from the Dirac current $\vec{J}_{\text{Dirac}} = c\,\Psi^\dagger\vec{\alpha}\,\Psi$, write the Dirac spinor in two components: $\Psi = \begin{pmatrix}\chi\\ \phi\end{pmatrix}$, so that

$$\vec{J}_{\text{Dirac}} = c\,(\chi^\dagger,\phi^\dagger)\begin{pmatrix}0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{pmatrix}\begin{pmatrix}\chi\\ \phi\end{pmatrix} = c\,(\chi^\dagger\,\vec{\sigma}\,\phi + \phi^\dagger\,\vec{\sigma}\,\chi). \quad (81)$$

In the non-relativistic regime we have (73) $\phi = \frac{c(\vec{\sigma}\cdot\vec{p})}{E+mc^2}\,\chi \approx \frac{c(\vec{\sigma}\cdot\vec{p})}{2mc^2}\,\chi$, with $E \approx mc^2$, $E+mc^2 \approx 2mc^2$, and similarly for $\phi^\dagger$. Substituting gives

$$\vec{J}_{\text{Dirac}} \approx \chi^\dagger\,\vec{\sigma}\,\frac{\vec{\sigma}\cdot\vec{p}}{2m}\chi + \frac{\chi^\dagger(\vec{\sigma}\cdot\vec{p})^\dagger}{2m}\vec{\sigma}\,\chi \quad (82)$$

$$= \frac{1}{m}\,\text{Re}\{\chi^\dagger\,\vec{p}\,\chi\} + \frac{\hbar}{2m}\,\nabla\times(\chi^\dagger\vec{\sigma}\chi). \quad (83)$$

Here we used the identity $\sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k + \delta_{ij}$, and using the chain rule for the curl term you recover the former expression. Therefore, with electromagnetic fields $\hat{\pi} = \frac{\hbar}{i}\nabla - q\vec{A}$, the Pauli current reads

$$\vec{J}_{\text{Pauli}} = \frac{1}{m}\,\text{Re}\{\chi^\dagger[\tfrac{\hbar}{i}\nabla - q\vec{A}]\chi\} + \frac{\hbar}{2m}\,\nabla\times(\chi^\dagger\vec{\sigma}\chi). \quad (84)$$

To read more about this extra term, see [4]. You may have noticed we did not use this term when computing the Pauli current for the Landau levels, in that case it did not matter as the stationary states were eigenstates of S_z. Moreover, this term does not contribute to the divergence $\boldsymbol{\nabla}\cdot J$, since $\boldsymbol{\nabla}\cdot\left(\nabla\times\vec{C}\right) = 0$, and should be understood as a current between different spin states in a fixed position $\vec{x}$, therefore it does not carry probability from a point in space to another.
The way we derive the probability current in section X A is incomplete, since we can sum the rotational of a vector, and get the same continuity equation. Hence, is it only possible to obtain a well-defined expression, taking the non-relativistic limit of the Dirac probability current.

XV. HALL EFFECT

We now have a magnetic field in the z-direction and an electric field in the negative x-direction:

$$\vec{B} = B\,\hat{z}, \qquad \vec{E} = -E\,\hat{x}.$$

Choosing the gauge potentials

$$A^0 = E\,x, \quad A^1 = 0, \quad A^2 = B\,x, \quad A^3 = 0,$$

so that $A^\mu = (A^0, A^1, A^2, A^3) = (Ex, 0, Bx, 0)$. This is called the Landau gauge .

The Pauli Hamiltonian is

$$\hat{H}_{\text{Pauli}} = \frac{(\vec{\sigma}\cdot\vec{\pi})^2}{2m} + qA^0 = \frac{(\hat{p}-q\,\vec{A})^2}{2m} - \frac{q\hbar}{2m}\,\vec{\sigma}\cdot\vec{B} + q\,A^0. \quad (85)$$

Substituting $\vec{A} = (0, Bx, 0)$ and $A^0 = Ex$ and restricting to the xy-plane ($\hat{p}_z = 0$) gives

$$\hat{H}_{\text{Pauli}} = \frac{\hat{p}_x^2 + (\hat{p}_y - qBx)^2}{2m} - \frac{q\hbar}{2m}\,\sigma_z\,B + q\,E\,x. \quad (86)$$

Since $[\hat{H}_{\text{Pauli}}, \hat{p}_y] = 0$, eigenfunctions can be chosen as

$$\Psi(x,y,z) = \chi(x)\,e^{ik_y y}\,e^{ik_z z}.$$

Ignoring the z-direction ($k_z = 0$) and confining to the plane yields

$$\Psi(x,y) = \chi(x)\,e^{ik_y y}.$$

The total Hamiltonian separates as

$$\hat{H} = \hat{H}_{\text{orb}} + \hat{H}_{\text{spin}}. \quad (87)$$

Explicitly,

$$\hat{H}_{\text{orb}} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} - \frac{qBx}{m}\,\hat{p}_y + \frac{q^2B^2x^2}{2m} + qEx, \quad (88)$$

$$\hat{H}_{\text{spin}} = -\omega_B\,\hat{S}_z. \quad (89)$$

Since $[\hat{H}_{\text{Pauli}}, \hat{p}_y] = 0$, we set $\hat{p}_y \to \hbar k_y$. Then

$$\hat{H}_{\text{orb}} = \frac{\hat{p}_x^2}{2m} + \frac{\hbar^2k_y^2}{2m} + \frac{qE - qB\hbar k_y}{m}\,x + \frac{q^2B^2x^2}{2m}. \quad (90)$$

Completing the square in x:

$$\hat{H}_{\rm orb} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2m}\Big(qBx - \hbar k_y + \frac{mE}{B}\Big)^2 - \frac{mE^2}{2B^2} + \frac{\hbar k_y E}{B}. \tag{91}$$

This is a shifted harmonic oscillator plus constant offset, whose eigenvalues and eigenfunctions follow immediately. Setting

$$\omega_B = \frac{qB}{m}, \qquad x_0 = \frac{\hbar k_y}{qB} - \frac{mE}{qB^2}.$$

The orbital eigenstates $|n_x, k_y\rangle$ thus have energies

$$E_{n_x,k_y} = \hbar\omega_B\Big(n_x + \tfrac{1}{2}\Big) - \frac{mE^2}{2B^2} + \frac{\hbar k_y E}{B}.$$

This looks very similar to the results we obtained for the Landau levels, but in this case the energy does depend on k_y.

The spin Hamiltonian $\hat{H}_{\rm spin} = -\omega_B \hat{S}_z$ has eigenvectors $|\eta\rangle$ ($\eta = \pm 1$) with eigenvalues

$$\hat{H}_{\rm spin}\,|\eta\rangle = -\eta\,\frac{\hbar\omega_B}{2}\,|\eta\rangle.$$

Therefore, the total eigenstates $|n_x, k_y, \eta\rangle$ satisfy

$$\hat{H}\,|n_x, k_y, \eta\rangle = \Big[\hbar\omega_B\big(n_x + \tfrac{1}{2}\big) - \eta\,\tfrac{\hbar\omega_B}{2} - \tfrac{mE^2}{2B^2} + \tfrac{\hbar k_y E}{B}\Big]\,|n_x, k_y, \eta\rangle.$$

So we get the same that for the Landau levels, the spin splits in two the energy levels at the same distance ($\hbar\omega$) that the intervals between n_x levels, and again we have a fundamental level that is non-degenerate.

XVI. PROBABILITY CURRENT IN THE HALL EFFECT

We now study the probability current of an eigenstate $|n_x, k_y, \eta\rangle$ in the Hall configuration. The Pauli current is

$$\vec{J}_{\rm Pauli} = \frac{1}{m}\,\mathrm{Re}\{\chi^\dagger[\tfrac{\hbar}{i}\nabla - q\vec{A}]\chi\} + \frac{\hbar}{2m}\nabla\times(\chi^\dagger\vec{\sigma}\chi). \tag{92}$$

For the state,

$$\chi = \begin{pmatrix}\psi_{n_x,k_y}(x)\\ 0\end{pmatrix}, \quad \psi_{n_x,k_y}(x) = \varphi_{n_x}(x - x_0)e^{ik_y y},$$

only the upper component is nonzero. Thus

$$\begin{aligned}\frac{\hbar}{i}\chi^\dagger\nabla\chi &= \frac{\hbar}{i}\big(\psi^*\partial_x\psi,\ \psi^*\partial_y\psi,\ 0\big)\\ &= \frac{\hbar}{i}\varphi_{n_x}(x - x_0)\,(\partial_x\varphi_{n_x},\ ik_y\varphi_{n_x},\ 0),\end{aligned}$$

and

$$q\chi^\dagger\vec{A}\chi = \big(0,\ q\varphi_{n_x}(x - x_0)^2 Bx,\ 0\big). \tag{93}$$

Taking the real part,

$$\mathrm{Re}\ \chi^\dagger\big[\tfrac{\hbar}{i}\nabla - q\vec{A}\big]\chi = \big(0,\ \hbar k_y\varphi_{n_x}^2 - qBx\varphi_{n_x}^2,\ 0\big). \tag{94}$$

The spin-magnetization density is

$$\chi^\dagger\vec{\sigma}\chi = \hat{k}\,\varphi_{n_x}(x - x_0)^2. \tag{95}$$

Hence its curl is

$$\nabla\times\big(\chi^\dagger\vec{\sigma}\chi\big) = \begin{vmatrix}\hat{i} & \hat{j} & \hat{k}\\ \partial_x & \partial_y & \partial_z\\ 0 & 0 & \varphi_{n_x}^2\end{vmatrix} = \hat{i}\,\partial_y\big(\varphi_{n_x}^2\big) - \hat{j}\,\partial_x\big(\varphi_{n_x}^2\big). \tag{96}$$

But the first term is null, thus $\nabla\times\big(\chi^\dagger\vec{\sigma}\chi\big) = -\,\hat{j}\,\partial_x\big(\varphi_{n_x}^2\big)$. Therefore the full Pauli current in the Hall effect becomes

$$\vec{J}_{\rm Pauli} = \big(0,\ \tfrac{\hbar k_y - qBx}{m}\,\varphi_{n_x}^2 - \tfrac{\hbar}{2m}\,\partial_x(\varphi_{n_x}^2),\ 0\big).$$

Hence, the spin term actually contributes to the probability current (see [4]). x

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