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Landau level quantization of Dirac electrons on the sphere

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ABSTRACT

Interactions in Landau levels can stabilize new phases of matter, such as fractionally quantized Hall states. Numerical studies of these systems mostly require compact manifolds like the sphere or a torus. For massive dispersions, a formalism for the lowest Landau level on the sphere was introduced by Haldane (1983). Graphene and surfaces of 3D topological insulators, however, display massless (Dirac) dispersions, and hence require a different description. We generalize a formalism previously developed for Dirac electrons on the sphere in zero field to include the effect of an external, uniform magnetic field.

Progress in theoretical physics has always been achieved through the interplay of obtaining experimental data with comparing it to the predictions of the ideas, concepts, and theories suggested to explain the data. In earlier periods, the implications of theoretical models could be explored only through analytic calculations. During the past four decades, however, the availability of ever more powerful computers has significantly reshaped this process. Among early highlights were the development of the renormalization group by Wilson [1], the discovery of universality in the onset of chaos by Feigenbaum [2], and the formulation of Laughlin's wave function for fractional quantized Hall liquids [3]. Laughlin's discovery is particularly striking in this context as it was guided by a numerical experiment [4]. Laughlin numerically diagonalized a system of a few electrons in the lowest Landau level in the open plane, and observed that the canonical angular momentum of the ground state jumped by a factor of three upon turning on a strong repulsive interaction. The experimental discovery of the effect had inspired the numerical experiment, and the numerical experiment provided the crucial hint to the formulation of the theory. The theory was only accepted by the community at large after Haldane formulated it on a sphere [5], a geometry without a boundary and hence without gapless edge modes, and showed that Laughlin's trial state can be adiabatically connected to the

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ground state for Coulomb interactions without closure of the energy gap [6]. A more recent example for the importance of numerical experiments is the discovery of the topological insulator (TI) as a consequence of band inversion by Kane and Mele [7,8], a phase which was subsequently realized in HgTe quantum wells [9,10].

The efficient implementation of numerical experiments often requires geometries which cannot be realized in a laboratory, such as periodic boundary conditions (PBCs). When the underlying lattice plays no role in the effective model one wishes to study, the simplest geometry without a boundary is the sphere. It continues to be of seminal importance in numerical studies of quantized Hall states and other states of matter in two dimensional electron gases subject to a magnetic field. While most of the work on TIs focusses on the single particle description of topologically non-trivial band structures, the most promising avenues to observe topologically non-trivial many body condensates in this context may be at the surface of a 3D TI [11,12]. The single particle states on these surfaces are described by a single Dirac cone, which would be impossible to realize on a lattice due to the fermion doubling theorem [13]. Even as a continuum theory, coupling the electrons minimally to the electromagnetic gauge field requires an even number of Dirac cones, or an axion term on one side of the surface [14]. In other words, a single Dirac cone at a surface requires a termination of a topological insulator [15]. The situation is less intricate in graphene, where a 2D lattice not embedded in a 3D topological structure features one Dirac cones per spin and valley degree of freedom, and hence a total of four cones [16].

Regarding the numerical study of interaction effects on surfaces of 3D TIs, the only work published so far has employed a spherical geometry [17,18]. (For PBCs, the numerics is far more challenging, and the studies performed so far are unpublished as of yet [19].) To formulate the single particle Hilbert space for the single Dirac cone on the sphere, we employed a formalism introduced earlier by one of us [20] to describe Landau levels (LLs) for massive electrons on the sphere, which in turn generalized the spinor coordinate formalism introduced earlier by Haldane [5] for the lowest LL. The magnetic monopole in the center of the sphere, of monopole charge $2s_0 = +1$ for $\uparrow$ spins and $2s_0 = -1$ for $\downarrow$ spins, emerges from the Berry's phase associated with rotations of the reference system for the spin. (In our notation, spin $\uparrow$ and $\downarrow$ refer to spin directions normal to the surface of the sphere.) We obtained the single particle Hamiltonian,

$$H = \frac{\hbar v}{R}\begin{pmatrix} 0 & -S^{+} \\ -S^{-} & 0 \end{pmatrix}, \tag{1}$$

where the angular momentum operators S^- and S^+ effectively act as LL "raising" and "lowering" operators on the sphere, v is the Dirac velocity, and R the radius of the sphere. This form resembles the single particle Hamiltonian for Dirac electrons subject to a uniform magnetic field $\boldsymbol{B} = -B\boldsymbol{e}_z$ in the plane,

$$H = \frac{\hbar v\sqrt{2}}{l}\begin{pmatrix} 0 & ia^{\dagger} \\ -ia & 0 \end{pmatrix}, \tag{2}$$

where $a^\dagger$ and a are Landau level raising and lowering operators (see Refs. [21] or [22] for reviews of the formalism), and $l = \sqrt{\frac{\hbar c}{eB}}$ is the magnetic length.

In this paper, we first provide a more detailed derivation of (1) than space allowed in Ref. [17], and second, show that (1) also holds in the presence of an external, radial magnetic field $\boldsymbol{B} = B\boldsymbol{e}_{\mathrm{r}}$ supplementing the Berry flux. We assume a field strength $B = 2b_0\Phi_0/4\pi R^2$, where $\Phi_0 = 2\pi\hbar c/e$ with $e > 0$ is the Dirac flux quantum, such that the total number of Dirac flux quanta through the surface is $2b_0$. *The only change due to the field is that the $\uparrow$ and $\downarrow$ spin components of the spinor ψ^{λ}_{nm},*

$$H\psi^{\lambda}_{nm} = E_n\psi^{\lambda}_{nm}, \quad \psi^{\lambda}_{nm} = \begin{pmatrix} \phi^{\uparrow}_{nm} \\ \lambda\phi^{\downarrow}_{nm} \end{pmatrix}, \tag{3}$$

are given by (massive) LL wave functions [20] corresponding to total magnetic flux $\Phi = (2b_0 \pm 1)\Phi_0$ rather than just $\pm\Phi_0$ through the surface of the sphere, and the energies for states in (Dirac) LL n are given by

$$E_n = \lambda\frac{\hbar v}{R}\sqrt{(2b_0 + n)n} \tag{4}$$

rather than $E_n = \lambda \frac{\hbar v}{R} n$. $\lambda = \pm 1$ distinguishes positive from negative energy solutions. (Note that since the level $n = 0$ does not exist for the zero field case, n is shifted by one as compared to the discussion in Ref. [17].)

Let us now turn to the details of the derivation. We consider the Dirac Hamiltonian

$$H = \hbar v \hat{\boldsymbol{n}} \left[\left(-\mathrm{i}\nabla - \frac{e}{c}\boldsymbol{A} \right) \times \boldsymbol{\sigma} \right], \tag{5}$$

where $\hat{\boldsymbol{n}}$ is the surface normal, and $\boldsymbol{A}$ the vector potential generating the external magnetic field. Note that the scalar product with the surface normal ensures a rotationally symmetric form of the 2D Dirac (surface) Hamiltonian. For the surface states of a 3D TI, $\boldsymbol{\sigma} = (\sigma_\mathrm{x}, \sigma_\mathrm{y}, \sigma_\mathrm{z})$ is twice the physical electron spin vector. For graphene ($\hat{\boldsymbol{n}} = \hat{\boldsymbol{z}}$), the Pauli matrices act on the two-dimensional space spanned by the two sites contained in the unit cell of the hexagonal lattice, usually denoted as sublattice A and B. In the case of the TI, the external magnetic field will also couple to the electron spin via a Zeeman term, but since this will not give rise to any conceptual difficulties, we will only address it briefly after the derivation. In the following, we set $\hbar = c = 1$.

In the absence of the external magnetic field, Imura et al. [23] used the example of a 3D TI to show that on a sphere with radius R, (5) becomes

$$H_0 = \frac{v}{R} \left(\sigma_\mathrm{x} \Lambda_\theta + \sigma_\mathrm{y} \Lambda_\phi \right), \tag{6}$$

where

$$\boldsymbol{\Lambda} = -i \left[\boldsymbol{e}_\varphi \partial_\theta - \boldsymbol{e}_\theta \frac{1}{\sin\theta} \left(\partial_\varphi - \frac{\mathrm{i}}{2} \sigma_\mathrm{z} \cos\theta \right) \right] \tag{7}$$

is the dynamical angular momentum of an electron in the presence of a magnetic monopole with strength $2\pi\sigma_\mathrm{z}$, and (r, θ, φ) are spherical coordinates. The monopole strength or Berry flux through the sphere is hence $\pm 2\pi$ for $\uparrow$ spins and $\downarrow$ spins respectively (i.e., spins pointing in the $\pm\boldsymbol{e}_\mathrm{r}$ direction). The origin of this Berry phase is easily understood. Since the coordinate system for our spins (to which our Pauli matrices $\sigma_\mathrm{x}, \sigma_\mathrm{y}, \sigma_\mathrm{z}$ refer to) is spanned by $\boldsymbol{e}_\theta, \boldsymbol{e}_\varphi, \boldsymbol{e}_\mathrm{r}$, it will rotate as the electron is taken around the sphere. For general trajectories, the Berry phase generated by this rotation is given by $\pm\frac{1}{2}$ times the solid angle subtended by the trajectory. Formally, this phase is generated by a monopole with strength $\pm 2\pi$ at the origin for $\uparrow$ and $\downarrow$ spins, respectively. Substitution of (7) into (6) yields

$$H = \frac{v}{R} h, \quad h = \begin{pmatrix} 0 & h^+ \\ h^- & 0 \end{pmatrix}, \tag{8}$$

with

$$h^\pm = h_0^\pm = \mp \left(\partial_\theta + \frac{1}{2}\cot\theta \right) + \frac{\mathrm{i}\partial_\varphi}{\sin\theta}. \tag{9}$$

Even though Imura et al. [23] derived (8) with (9) discussing the surface termination of a 3D TI, it is by no means specific to this setting, as *the Berry phase is a general property of the Dirac Hamiltonian on a curved surface.* To illustrate this point, we will derive (8) with (9) now directly from (5) with $\boldsymbol{A} = 0$.

On a sphere with fixed radius R, the nabla operator in spherical coordinates reads

$$\nabla = \frac{1}{R} \left(\boldsymbol{e}_\theta \partial_\theta + \boldsymbol{e}_\varphi \frac{\partial_\varphi}{\sin\theta} \right). \tag{10}$$

This form, however, is not suited for direct substitution into (5), since $-\mathrm{i}\nabla$ has to be hermitian, while

$$(\partial_\theta)^\dagger = -(\partial_\theta + \cot\theta), \quad (\partial_\varphi)^\dagger = -\partial_\varphi. \tag{11}$$

(The solid angle measure $d\Omega = d\theta d\phi \sin\theta$ gives rise to the $\cot\theta$ term when we go from $\psi_\mathrm{a}^* \partial_\theta \psi_b$ to $-(\partial_\theta \psi_\mathrm{a}^*)\psi_b$ via partial integration.) If we then substitute the hermitian combination $\frac{1}{2}\big((-\mathrm{i}\nabla) + (-\mathrm{i}\nabla)^\dagger\big)$ and $\boldsymbol{\sigma} = \boldsymbol{e}_\theta \sigma_\mathrm{x} + \boldsymbol{e}_\varphi \sigma_\mathrm{y} + \boldsymbol{e}_\mathrm{r} \sigma_\mathrm{z}$ into (5), we obtain (8) with (9).

To include the external magnetic field, we choose the latitudinal gauge

$$\boldsymbol{A} = -\boldsymbol{e}_\varphi \frac{b_0}{eR} \cot\theta. \tag{12}$$

The singularities of $\boldsymbol{B} = \nabla \times \boldsymbol{A}$ at the poles are without physical significance. They describe infinitely thin solenoids admitting flux $b_0 \Phi_0$ each, exist for the Berry connection as well, and reflect our inability to formulate true magnetic monopoles.

Substitution of (12) into (5) yields (8) with

$$\begin{aligned} h^{\pm} &= h_0^{\pm} + b_0 \cot\theta \\ &= \mp \partial_\theta + \left(b_0 \mp \frac{1}{2}\right) \cot\theta + \frac{\mathrm{i}\partial_\varphi}{\sin\theta}. \end{aligned} \tag{13}$$

As in the zero field case, (8) with (13) describes a "Dirac Hamiltonian" in the sense that

$$\begin{aligned} h^2 &= \begin{pmatrix} h^+h^- & 0 \\ 0 & h^-h^+ \end{pmatrix} \\ &= \begin{pmatrix} \Lambda_{s_0}^2 + s_0\big|_{s_0=b_0+\frac{1}{2}} & 0 \\ 0 & \Lambda_{s_0}^2 - s_0\big|_{s_0=b_0-\frac{1}{2}} \end{pmatrix} \end{aligned} \tag{14}$$

is diagonal. Apart from an overall numerical factor,

$$\Lambda_{s_0}^2 = -\frac{1}{\sin\theta}\partial_\theta \left(\sin\theta\, \partial_\theta\right) - \frac{1}{\sin^2\theta}\left(\partial_\varphi - \mathrm{i}s_0\cos\theta\right)^2 \tag{15}$$

is the Hamiltonian of a massive electron moving on a sphere with a monopole of strength $4\pi s_0$ in the center [5]. The LLs for massive electrons on the sphere are spanned by two mutually commuting SU(2) algebras [20], one for the cyclotron momentum ($\boldsymbol{S}$) and one for the guiding center momentum ($\boldsymbol{L}$). The Casimir of both is given by $\boldsymbol{L}^2 = \boldsymbol{S}^2 = s(s+1)$, where $s = |s_0| + n$ and $n = 0, 1, \ldots$ is the LL index for massive electrons.

With $\Lambda^2 = \boldsymbol{L}^2 - s_0^2$, we obtain

$$\Lambda_{s_0}^2 \pm s_0\big|_{s_0=b_0\pm\frac{1}{2}} = \begin{cases} (2b_0 + n_\uparrow + 1)(n_\uparrow + 1), \\ (2b_0 + n_\downarrow)n_\downarrow, \end{cases} \tag{16}$$

for the diagonal elements of $\uparrow$ and $\downarrow$ spins in (14). The $\uparrow$ spin components $\phi_{nm}^{\uparrow}$ are hence described by massive LL wave functions in level $n_\uparrow = n - 1$ if the $\downarrow$ spin components $\phi_{nm}^{\downarrow}$ are described by massive LL wave functions in level $n_\downarrow = n$, with $s = b_0 + n - \frac{1}{2}$ for both. The eigenvalues of h^2 are given by $\varepsilon_n^2 = (2b_0 + n)n$.

In terms of the spinor coordinates

$$u = \cos\frac{\theta}{2} e^{i\frac{\varphi}{2}},\ \ v = \sin\frac{\theta}{2} e^{-i\frac{\varphi}{2}}, \tag{17}$$

introduced by Haldane [5], and their complex conjugates $\bar{u}, \bar{v}$,

$$\begin{aligned} S^x + iS^y = S^+ &= u\partial_{\bar{v}} - v\partial_{\bar{u}}, \\ S^x - iS^y = S^- &= \bar{v}\partial_u - \bar{u}\partial_v, \\ S^z &= \frac{1}{2}(u\partial_u + v\partial_v - \bar{u}\partial_{\bar{u}} - \bar{v}\partial_{\bar{v}}), \end{aligned} \tag{18}$$

$$\begin{aligned} L^x + iL^y = L^+ &= u\partial_v - \bar{v}\partial_{\bar{u}}, \\ L^x - iL^y = L^- &= v\partial_u - \bar{u}\partial_{\bar{v}}, \\ L^z &= \frac{1}{2}(u\partial_u - v\partial_v - \bar{u}\partial_{\bar{u}} + \bar{v}\partial_{\bar{v}}). \end{aligned} \tag{19}$$

The physical Hilbert space is restricted to states with S^z eigenvalue s_0 [20]. For our spin component wave functions, this restriction reads

$$S^z\phi_{nm}^{\uparrow} = \left(b_0 + \frac{1}{2}\right)\phi_{nm}^{\uparrow},\ \ S^z\phi_{nm}^{\downarrow} = \left(b_0 - \frac{1}{2}\right)\phi_{nm}^{\downarrow}. \tag{20}$$

The greatly simplifying observation is now that for massive LL wave functions subject to (20),

$$h^+\phi^{\downarrow}_{nm} = -S^+\phi^{\downarrow}_{nm}, \quad h^-\phi^{\uparrow}_{nm} = -S^-\phi^{\uparrow}_{nm}, \tag{21}$$

and hence that

$$h = \begin{pmatrix} 0 & -S^+ \\ -S^- & 0 \end{pmatrix}. \tag{22}$$

We now verify the first equation in (21) by explicit evaluation of $h^+\phi^{\downarrow}_{nm}$. $\phi^{\downarrow}_{nm}$ has to take the form of a massive Landau level wave function [20]

$$\phi^{\downarrow}_{nm} \sim (L^-)^{s-m}(S^-)^n u^{2s} \sim (L^-)^{s-m}\, \bar{v}^n u^{2s-n}$$

with $s = b_0 + n - \frac{1}{2}$. Upon expansion we obtain terms of the form

$$\begin{aligned}\chi^{\downarrow}_q &= v^{s-m-q}\, \bar{v}^{n-q}\, \bar{u}^q\, u^{s-n+m+q} \\ &= \left(\sin\frac{\theta}{2}\right)^{s+n-m-2q} \left(\cos\frac{\theta}{2}\right)^{s-n+m+2q} e^{\mathrm{i}m\varphi}\end{aligned}$$

with $q = 0, \ldots, s-m$. Rewriting (13) as

$$h^{\pm} = \mp\,\partial_\theta + \left(b_0 \mp \frac{1}{2} + \mathrm{i}\partial_\varphi\right)\cot\frac{\theta}{2} - \left(b_0 \mp \frac{1}{2} - \mathrm{i}\partial_\varphi\right)\tan\frac{\theta}{2},$$

we easily find

$$h^+\chi^{\downarrow}_q = \left[-(n-q)\cot\frac{\theta}{2} + q\tan\frac{\theta}{2}\right]\chi^{\downarrow}_q,$$

which is equal to $-S^+\chi^{\downarrow}_q$. The second equation in (21) is shown along the same lines.

The Dirac property of h, the eigenvalues of h^2, the massive LL form of the component wave functions of the Dirac spinor, and finally (22) imply

$$h\psi^{\lambda}_{nm} = \lambda\sqrt{(2b_0+n)n}\,\psi^{\lambda}_{nm}, \quad \psi^{\lambda}_{nm} = \begin{pmatrix} \phi^{\uparrow}_{nm} \\ \lambda\phi^{\downarrow}_{nm} \end{pmatrix}, \tag{23}$$

where $\lambda = \pm 1$ distinguishes positive and negative energy solutions, and m is the eigenvalue of L^{z}. The (only relatively normalized) component wave functions are given by

$$\phi^{\uparrow}_{nm} = \sqrt{n}\,(L^-)^{s-m}\,\bar{v}^{n-1}u^{2s+1-n}, \tag{24}$$

$$\phi^{\downarrow}_{nm} = -\sqrt{2b_0+n}\,(L^-)^{s-m}\,\bar{v}^n u^{2s-n}, \tag{25}$$

where $s = b_0 + n - \frac{1}{2}$ and $m = -s, -s+1, \ldots, s$. The degeneracy in each Dirac LL is hence $2s+1 = 2(b_0+n)$. The level $n = 0$ with dimensionless energy $\varepsilon_0 = 0$ is completely spin polarized, with the spins aligned in the direction of $-\boldsymbol{B}$ as $\phi^{\uparrow}_{0m} = 0$; this level does not exist for the zero field case elaborated in Ref. [17]. In all other levels, the single particle states have equal amplitudes for $\uparrow$ and $\downarrow$ spins.

To gain further insight into the single particle wave functions, consider the fully normalized spinors for $m = s$, i.e., for states localized at the north pole of the sphere,

$$\begin{aligned}\psi^{\lambda}_{ns} = &\sqrt{\frac{1}{2}\binom{2(b_0+n)}{n}} \cdot \left(\sin\frac{\theta}{2}\right)^{n-1} \left(\cos\frac{\theta}{2}\right)^{2b_0+n-1} \\ &\cdot \begin{pmatrix} \sqrt{n}\,\cos\dfrac{\theta}{2} \\ -\lambda\sqrt{2b_0+n}\,\sin\dfrac{\theta}{2} \end{pmatrix}.\end{aligned} \tag{26}$$

We see that for $n \neq 0$, the spins are aligned with the magnetic field at the pole, and then turn in the $\sigma_{\mathrm{x}}, \sigma_{\mathrm{z}}$ plane spanned by $\boldsymbol{e}_\theta$ and $\boldsymbol{e}_{\mathrm{r}}$ until they point in the direction opposing the magnetic field far away from the pole. Almost all the amplitude is contained in narrow rings, which have their maximal amplitudes at

$$\left(\tan\frac{\theta}{2}\right)^4 = \frac{n(n-1)}{(2b_0+n)(2b_0+n-1)}. \tag{27}$$

This concludes our derivation of LL quantization for Dirac fermions on the sphere as applicable to graphene.

For the surfaces of 3D TIs, the spin in (5) is the physical electron spin, which also couples to the magnetic field via a Zeeman term,

$$H_{\mathrm{B}} = -\frac{1}{2} g_{\mathrm{s}} \mu_{\mathrm{B}} B \sigma_{\mathrm{z}}, \tag{28}$$

where μ_{B} is the Bohr magneton, and g_{s} the Landé g-factor. Even though it is only a small correction in actual TI surface states, we briefly address it here. For $n = 0$, the Dirac LL is completely spin polarized and ψ_{nm}^{λ} with (24) and (25) is an eigenstate of (28). The energy is given by

$$E_0 = -\frac{1}{2} g_{\mathrm{s}} \mu_{\mathrm{B}} B. \tag{29}$$

For $n \neq 0$, let the spinor $(\alpha, \beta)^{\mathrm{T}}$ refer to a combination of positive and negative energy solutions as given by (23) with (24) and (25), $\alpha\psi_{nm}^{+} + \beta\psi_{nm}^{-}$. In this two-dimensional space, the total Hamiltonian including (28) is given by

$$\tilde{H} = \frac{\hbar v}{R}\varepsilon_n \sigma_{\mathrm{z}} - \frac{1}{2} g_{\mathrm{s}} \mu_{\mathrm{B}} B \sigma_{\mathrm{x}}, \tag{30}$$

where $\varepsilon_n = \sqrt{(2b_0+n)n}$ is the absolute value of the dimensionless energy in the absence of the Zeeman field. This is again a "Dirac Hamiltonian" in the sense that the square is diagonal, which allows us to read off the energies

$$\tilde{E}_n = \lambda \sqrt{\left(\frac{\hbar v}{R}\right)^2 (2b_0+n)n + \left(\frac{1}{2} g_{\mathrm{s}} \mu_{\mathrm{B}} B\right)^2}, \tag{31}$$

where $\lambda = \pm 1$ again distinguishes positive and negative energy solutions. The eigenstates of (30) are given by

$$\tilde{\psi}_{nm}^{+} = \left(\frac{\hbar v}{R}\varepsilon_n + |\tilde{E}_n|\right)\psi_{nm}^{+} - \left(\frac{1}{2} g_{\mathrm{s}} \mu_{\mathrm{B}} B\right)\psi_{nm}^{-}, \tag{32}$$

$$\tilde{\psi}_{nm}^{-} = \left(\frac{1}{2} g_{\mathrm{s}} \mu_{\mathrm{B}} B\right)\psi_{nm}^{+} + \left(\frac{\hbar v}{R}\varepsilon_n + |\tilde{E}_n|\right)\psi_{nm}^{-}. \tag{33}$$

The Zeeman term hence yields only a small mixing of the positive and negative energy solution of the Dirac LLs (23) with (24) and (25).

In conclusion, we have presented a formalism for Landau level quantization of Dirac electrons in the spherical geometry. The formalism is largely identical to the formalism we introduced for Dirac electrons without an external magnetic field in Ref. [17], where the issue of Landau level quantization arose due to the Berry connection associated with the coupling of the Dirac spinor to the curvature of the sphere. Since the formalism is not limited to either zero field nor to surface states of 3D TIs, but applies to any other 2D system with Dirac cones such as graphene, the importance of it goes way beyond the immediate applications studied in Ref. [17].

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