Electron in the field of magnetic charge: Tight binding solution and mapping on a realistic physical system

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Electron in the field of a magnetic charge (the continuum formulation)

$$\mathbf{B} = rac{g}{r^2}\hat{\mathbf{r}}$$



Dirac (1931): If there is a magnetic charge g then g is quantized as:

$$\frac{2eg}{\hbar c} = 2S$$
 (an integer)

The flux of g through a close surface (e.g a sphere) is then calculated using Gauss theorem for magnetic charge

$$4\pi g = 2S\Phi_0 = 2S\frac{hc}{e}$$

Proofs: (Among others) T. T. Wu and C. N. Yang (1975) (defining non-singular vector potential) See also S. Coleman: Erice Lectures (1982). R. Jackiw (1982) Use only gauge invariant arguments. "The Dirac monopole: Again" R. Jackiw arXiv:hep-th/0212058 Electron in the field of monopole: Solutions in the continuum

Die verallgemeinerten Kugelfunktionen und die Wellenfunktionen eines Elektrons im Felde eines Magnetpoles.

Von Ig. Tamm in Moskau, zurzeit in Cambridge.

(Eingegangen am 26. Juni 1931.)

Saha (1936), S. Coleman Erice School (1982) $\mathbf{B} = \frac{g}{R^2} \hat{\mathbf{r}} = \frac{\hbar S}{eR^2} \hat{\mathbf{r}} = \nabla \times \mathbf{A}$ Hamiltonian $H = \frac{L^2}{2mR^2}$

 $\mathbf{L} = \mathbf{r} \times [-i\hbar \nabla + e\mathbf{A}(\mathbf{r})], \quad \mathbf{L} \cdot \mathbf{r} = 0, \text{ is NOT an angular momentum!}$

Generator of rotations $\mathbf{J} = \mathbf{L} + \hbar S \hat{\mathbf{r}}, \quad \mathbf{J} \cdot \hat{\mathbf{r}} = \hbar S$ $J^2 = \hbar^2 j(j+1), \quad j = S+l, \quad l = 0, 1, 2, \dots, \text{ and } 2S = n \text{ is an integer}$ Spectrum: $2mR^2H = J^2 - \hbar^2 S^2 = \hbar^2 [l(l+1) + (l+\frac{1}{2})2S]$

<u>Note</u>: spin-less particle with spin 1/2 angular momentum algebra!



How to define a vector potential on a sphere?? $\mathbf{A} = \frac{g}{R\sin\theta} (1 - \cos\theta)\phi$

The flux through the upper cap is

$$\Phi = \oint \mathbf{A} \cdot d\mathbf{s} = 2\pi g (1 - \cos \theta)$$

 $\theta \to \pi \Rightarrow \Phi = 4\pi q \text{ contour length} \to 0$

A must be singular

Solution: Wu & Yang(1975) Phase Factors $\frac{e}{\hbar c} \oint A_{\mu} dx^{\mu} \qquad f_{\mu\nu} \qquad e^{\frac{ie}{\hbar c}} \oint A_{\mu} dx^{\mu}$

phase (too much info) field(too little info) phase factor (exact info)

Fractional Quantization of the Hall Effect: A Hierarchy of Incompressible Quantum Fluid States

F. D. M. Haldane

The technical innovation that I make is to place a 2D electron gas of N particles on a spherical surface of radius R, in a radial (monopole) magnetic field $B = \hbar S/eR^2$ (>0) where 2S, the total magnetic flux through the surface in units of the flux quantum $\Phi_0 = h/e$, is integral as required by Dirac's monopole quantization condition.⁶ This

arXiv:cond-mat/0310232 [ps, pdf, other]

Anomalous Hall Effect and Magnetic Monopoles in Momentum-Space

Z. Fang, N. Nagaosa, K. S. Takahashi, A. Asamitsu, R. Mathieu, T. Ogasawara, H. Yamada, M. Kawasaki, Y. Tokura, K. Terakura Science 302N5642 (2003) 92-95

Nature 2007

Magnetic Monopoles in Spin Ice

C. Castelnovo¹, R. Moessner^{1,2}, and S. L. Sondhi³

11 more papers in cond-mat between 2000–2009

The automatic response of a CM physicist: Put the problem on a lattice !!

Tight binding model



Example: tight-binding model for electron hopping on the sphere in a central field. The TB is realized by the sites of the

Fullerene. (but we will start with simpler constructions).

The fields considered here are those of

I Magnetic charge

II Electric charge.

Note: No disorder, No e-e interaction, No TD limit.
Just the spectrum of a relatively small system
(hence the spectrum is discrete and finite).
As for magnetic charge: What is the motivation???
One answer: The beauty of the physics, or

Physical - Beauty



But here we will see that there is another motivation: In the tight binding version, the monopole problem can be mapped on a realistic system whose spectrum is the same.

In other words, once we measure the spectrum of an experimentally accessible system we can tell what would be the spectrum of a monopole system

So there will be no more apologies

Spectrum of electron on the plane with a perpendicular Mag. Field. Continuous (down) and lattice - Hofstadter-Azbel butterfly (right)



How to design sites for tight-binding on the sphere? Certainly not as in the Globe!! We want highest symmetry lattice: Platonic solids





p=coordination # q=# of links/face V=# of sites, L=# of links, F=# of faces

polyhedron	p	q	V	L	F
tetrahedron	3	3	4	6	4
cube	3	4	8	12	6
octahedron	4	3	6	12	8
dodecahedron	3	5	20	30	12
icosahedron	5	3	12	30	20

(L=F+V-2 by Euler's theorem) Tight binding Hamiltonian $H = \sum_{\langle n,m \rangle} a_n^{\dagger} e^{i\phi_{nm}} a_m + h.c$

How to choose the hopping phase factors???



$$H = \sum_{\langle n,m \rangle} a_n^{\dagger} e^{i\phi_{nm}} a_m + h.c$$

How to determine the hopping terms? The standard procedure is: Choose A, then compute the line integral of A along links of a face to get the flux per face. Then sum the fluxes on all faces to get the total flux.

$$2\pi \frac{\Phi_{\text{face}}}{\Phi_0} = \frac{e}{\hbar c} \sum_{\text{links}} \int_{\text{link}} \mathbf{A}_{\text{link}} \cdot d\mathbf{s}$$

This does not work for closed surfaces. Using the tetrahedron as an example:



but faces can have the same phase factors $e^{i\phi}, e^{i\phi}, e^{i\phi}$, and $e^{-3i\phi} = e^{i\phi}$ **PROVIDED** ϕ **IS QUANTIZED!!** as $\phi = \frac{2n\pi}{F=4}$, or $\Phi = \frac{1}{F}n\Phi_0$

In summary: To construct the hopping term for a platonic solid of m faces we have to design phase factors along links such that

$$\prod_{\substack{link\in face}} e^{i\frac{e}{\hbar c}\int_{link}\mathbf{A}\cdot d\mathbf{x}} = e^{\frac{2n\pi i\Phi_0}{m}}$$

where n=0,1,...m-1 is the number of monopoles. Once this job is completed the hopping integrals are known and the TB Hamiltonian is perfectly defined. This task is trivial for the tetrahedron (as we saw) but becomes more complicated for the more complex objects. It requires some technique in graph theory called Spanning Tree







Tetrahedron

n	E	m
0	3	1
	-1	3
1,3	$\sqrt{3}$	2
	$-\sqrt{3}$	2
2	1	3
	-3	1

V=4, matrix=4x4, F=periodicity=4 Dimension of irreps of point group depend on n





EGS (exercise for graduate students): Why only the cube has $E \leftrightarrow -E$ symmetry?







The dimensions if the irreps of the point magnetic rotation group depend on n





ofstadter-Azbel Butterfly (from Yossi Avron site) Our Flying-bat





The Fullerene: V=60, F=32 (20 Hexagons+12 Pentagons), L=90, spanning tree



 $12\Omega_5 + 20\Omega_6 = 4\pi$

EGS prove that: $\cos \Omega_5 = \frac{54887 + 720\sqrt{5}}{59049}$ $\cos \Omega_6 = \frac{511 + 945\sqrt{5}}{2916}$ $\frac{\Omega_5}{\Omega_6} = \frac{0.295072}{0.451275} = 0.653863 \approx \frac{2}{3}$

For a given monopole number n we construct $\alpha = e^{in\frac{\Omega_5}{2}}, \beta = e^{in\frac{\Omega_6}{2}}$

The nontrivial phase factors we use are: $\alpha, \beta, \beta^2, \ \alpha^3 \beta^6, \ \alpha^6 \beta^{12}, \alpha^9 \beta^{16}$

Magic numbers at $Q = N \times 84$ because $84\Omega_5 \approx 2$, $84\Omega_6 \approx 3$.



Part (2)-electron on the sphere in a central field of electric charge

$$\mathbf{E} = rac{q}{r^2} \hat{\mathbf{r}}$$



E cannot push or pull the electron. The only effect is the spin-orbit interaction. In the continuous geometry (spherical shell) we get Atomic SO interaction L.S

From Pauli Equation: SO= $\sigma \times \mathbf{E} \cdot \mathbf{p} = \sigma \cdot \mathbf{E} \times \mathbf{p}$



Tight binding: Experimental realization??

It is possible now to put an atom (or Ion) at the center of a Fullerene Derivatives (Lantanocene, Yterbocene) and create a central electric field of a point charge



LaC_{82}



(a) Total valence electron density of <u>31</u>P at the center of C60 fullerene in a cross sectional plane containing the P atom. (b) Donor electron density of 31P in a diamond nanocrystallite shown in a (111) What is the tight binding version of **L.S**?

The answer is again related to phase factors

Instead of U(1) phase factors for electromagnetism

We will have SU(2) "phase factors" (2x2 unitary matrices) for SO interaction



Nearest neighbor hopping in U(1) and SU(2)

$$\begin{array}{ll} \bullet & & \bullet \\ \mathbf{j} & & & \bullet \\ U(1): & a_i^{\dagger} e^{i \frac{e}{\hbar c} \int_i^j \mathbf{A}_{U(1)} \cdot d\mathbf{s}} a_j \\ SU(2): & a_{i\sigma}^{\dagger} e^{i \frac{e}{\hbar c} \int_i^j \mathbf{A}_{SU(2)} \cdot d\mathbf{s}} a_{j\nu} \end{array}$$

Careful with SU(2) because:

(1) The integral depends on the choice of contour connecting sites i and j.(2) The integral needs to be path ordered because different terms at different points need not commute.

Point (2) is avoided in case the direction of $\mathbf{E}_{x}d\mathbf{s}$ remains the same along the path.



This is a $2V \times 2V$ matrix. The physics enters in μ (SO strengths) and σ (spin) The geometry enters in $\hat{\mathbf{n}}_{ij}$. This is the tight binding version of the atomic $\mathbf{L} \cdot \mathbf{S}$



Properties of the spectrum (periodic in μ with period 2 pi):

Kramers theorem: Hso conserves TR invariance. each level En is at least 2 fold degenerate. 3

The spectrum is periodic in μ although the object is not a single ring

Semi periodicity: $E_a(\mu) = -E_a(\mu + \pi)$

Somewhat less obvious symmetry:

Let A and B denote vectors to adjacent sites $\mathbf{A} \cdot \vec{\sigma} S_{\mathbf{AB}}(\Theta - \mu) = S_{\mathbf{AB}}(\mu) \mathbf{B} \cdot \vec{\sigma}$ $\cos \Theta = \frac{\mathbf{A} \cdot \mathbf{B}}{AB}, \quad \hat{\mathbf{n}} = \frac{\mathbf{A} \times \mathbf{B}}{AB}, \quad S(\mu) = e^{i\mu \hat{\mathbf{n}} \cdot \vec{\sigma}}$

2

1

0

-2

-3^L

0.2

0.4

0.6

 $\mu/(2\pi)$

0.8

1.0

 $\mu \leftrightarrow \Theta - \mu$ symmetry: $H_{SO}(\mu)$ and $H_{SO}(\Theta - \mu)$ have the same spectrum

Special symmetry points: $\mu_0 = \frac{\Theta}{2}$, $\mu_1 = \frac{\Theta}{2} + \pi$ are symmetry points.

This is remarkable: Physics and geometry combine together!





Octahedron

a	$E_a(\mu)$	m_a
1	$4\cos\mu$	2
2	$4\sin\mu$	2
3	$-2\sin\mu$	4
4	$-2\cos\mu$	4











(strength of Spin-Orbit potential)



$$H_{SO}(\mu = \frac{\Theta}{2}) \sim \begin{pmatrix} H_1 & 0\\ 0 & H_1^* \end{pmatrix} \quad H_1 = \sum_{\langle AB \rangle} t_{AB} a_A^{\dagger} a_B, \quad t_{AB} = e^{i\omega_{AB}}$$

Each VxV block violates TR but the 2Vx2V two block matrix respects TR invariance.

$$\cos\omega_{AB} = \frac{\cos\Theta + \cos\theta_A + \cos\theta_B + 1}{4\cos\frac{\Theta}{2}\cos\frac{\theta_A}{2}\cos\frac{\theta_B}{2}} \to t_{AB} = e^{i\frac{\Omega_{NAB}}{2}}$$

This is a variant of the Heron formula for the spherical triangle ANB. The phase of t_{AB} is half the area of the spherical Triangle ANB (N=North Pole)!

$$\cos \Theta = \frac{\mathbf{A} \cdot \mathbf{B}}{AB}$$
$$\prod_{L_{AB} \in Face} t_{AB} = e^{i\frac{\Omega_{Face}}{2}}$$
$$\prod_{Face} e^{i\frac{\Omega_{Face}}{2}} = e^{2i \times 1 \times 2\pi} = 1$$

so the product of all hopping terms is exp(2i|pi)=1. Exactly as the product of face phase factors in the monopole problem with n=1

An important consequence: The spectrum of the monopole system at n=1 (experimentally inaccessible) can be constructed through the spectrum of the SO system at the symmetry point (experimentally accessible)!!

Take home (instead of summary)

