Quaternionic states of matter from synthetic gauge fields

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Q-BEC with Hopf invariant  3D Q-analytic Landau level
Ref.
1) Y. Li, X. F. Zhou, C. Wu, arxiv1205.2162.

Other related work
3) Y. Li, K. Intrilligator, Y. Yu, C. Wu, PRB 85, 85132(2012).

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Outline

• **Real numbers → complex numbers → quaternions (Q).**

• **Bosons:** real (positive) BEC → complex BEC → Q-BEC

  unconventional symm. beyond the “no-node” theorem.

  p-wave BEC, and topological spin textures

• **Fermions:** Q-analytic Landau levels in 3D.

  harmonic potential + spin-orbit coupling

  Cauchy-Riemann-Fueter condition.

• **Complex quaternions:** 3D Landau levels of Dirac fermions.
History: how did people accept “i”?

• Not because of the “ridiculous” Eq. \( x^2 = -1 \), but solving the cubic Eq (Cardano formula).

\[
x^3 + px + q = 0 \quad \rightarrow \quad x_1 = c_1 + c_2, \quad x_{2,3} = c_1e^{\pm\frac{i\pi}{3}} + c_2e^{\mp\frac{i\pi}{3}}
\]

\[
c_{1,2} = \sqrt[3]{-\frac{q}{2} \pm \sqrt{\Delta}} \quad \text{discriminant:} \quad \Delta = \left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3
\]

• Start up with real coefficients, and end up with three real roots, but no way to avoid “i”.

\[
x^3 - 3x = 0 \quad \rightarrow \quad x_1 = 0, \quad x_{2,3} = \pm\sqrt{3}
\]

\[
\Delta = -1, \quad \sqrt{\Delta} = \sqrt{-1}!!!
\]
The beauty of complex and elegance

- 2D rotation: Gauss plane.

- Euler formula: \( e^{i\pi} = -1 \)

- Complex analysis based on complex analyticity:
  \[
  \frac{\partial g}{\partial x} + i \frac{\partial g}{\partial y} = 0
  \]
  \[
  \frac{1}{2\pi i} \int \frac{1}{z - z_0} \, dz \quad g(z) = g(z_0)
  \]

- Applications: algebra fundamental theorem; Riemann hypothesis – distributions of prime numbers.

Quantum mechanics: the most important quantity in Schrödinger Eq is not hbar but “i”.

\[
i\hbar \frac{\partial}{\partial t} \psi = H \psi
\]
Quaternion: a further extension

- Three imaginary units \(i, j, k\).

\[
q = x + yi + zj + uk \quad i^2 = j^2 = k^2 = -1
\]

- Division algebra: \(ab \neq 0 \iff a \neq 0, b \neq 0\)

- Hamilton: Non-commutative division algebra (3D rotation is non-commutative).

\[
ij = -ji = k; \quad jk = -kj = i; \quad ki = -ik = j
\]

- Q-analyticity (Cauchy- Futer integral)

\[
\frac{\partial f}{\partial x} + i \frac{\partial f}{\partial y} + j \frac{\partial f}{\partial z} + k \frac{\partial f}{\partial u} = 0 \quad \Rightarrow \quad \frac{1}{2\pi^2} \iiint \frac{1}{|q - q_0|^2} \frac{1}{(q - q_0)} Dq \quad f(q) = f(q_0)
\]
Quat ernion plaque: Hamilton 10/16/1843

Brougham bridge, Dublin

\[ i^2 = j^2 = k^2 = ijk = -1 \]

Here as he walked by on the 16th of October 1843, Sir William Rowan Hamilton in a flash of genius discovered the fundamental formula for quaternion multiplication:

\[ i^2 = j^2 = k^2 = ijk = -1 \]

& cut it on a stone of this bridge.
3D rotation as 1\textsuperscript{st} Hopf map

- Rotation axis $\hat{\Omega}$, rotation angle: $\gamma$.

- $\hat{\Omega}$: imaginary quaternion unit: $\omega(\hat{\Omega}) = i \sin \theta \cos \phi + j \sin \theta \sin \phi + k \cos \theta$

3D rotation: unit quaternion $q$: $q = \cos \frac{\gamma}{2} + \omega(\hat{\Omega}) \sin \frac{\gamma}{2} \in S^3$

2D rotation: unit complex phase

- 3D vector $r \rightarrow$ imaginary quaternion. $\vec{r} \Rightarrow xi + yj + zk$

- 3D rotation and Hopf map.

\[ \vec{r} = \hat{z} = k \]
\[ \vec{r}' = qkq^{-1} \]

1\textsuperscript{st} Hopf map

$q \in S^3$

$qkq^{-1} \in S^2$
• Real numbers $\rightarrow$ complex numbers $\rightarrow$ quaternions (Q).

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  $p$-wave BEC, and topological spin textures

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Conventional BECs based on positive numbers

• “No-node” theorem: many-body ground state wavefunctions of bosons in the coordinate representation are positive-definite.

\[ \psi(r_1, r_2, \ldots r_n) \geq 0 \]

• A ground state property valid under general conditions (no rotation).

\[ H = \sum_{i=1}^{N} -\frac{\hbar^2 \nabla_i^2}{2M} + \sum_{i=1}^{N} V_{ex}(\vec{r}_i) + \sum_{i<j}^{N} V_{int}(\vec{r}_i - \vec{r}_j) \]

• No-go: Conventional BEC CANNOT break time-reversal symm spontaneously.

R. P. Feynman
An intuitive proof

\[ \psi(r_1, r_2, \ldots r_n) \quad |\psi(r_1, r_2, \ldots r_n)| \quad \psi(r_1, r_2, \ldots r_n) > 0 \]

\[ \langle \psi | H | \psi \rangle = \int dr_1 \ldots dr_n \frac{\hbar^2}{2m} \sum_{i=1}^{n} |\nabla_i \psi(r_1, \ldots r_n)|^2 + |\psi(r_1, \ldots r_n)|^2 \sum_{i=1}^{n} U_{\text{ex}}(r_i) \]

+ \[|\psi(r_1, \ldots r_n)|^2 \sum_{i<j} V_{\text{int}}(r_i - r_j) \]

• More formally and rigorously, c.f. Perron-Frobenius theorem.
Conventional BEC (invariant under rotations, s-wave-like)

- “No-node” theorem forbids unconventional symmetries, say, p, d, etc.

- Cf. conventional superconductivity: the pair WF belongs to the trivial (s-wave) representation of the rotation group.

\[ \Delta(r_1 - r_2) = \int d\vec{k} e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} \Delta(\vec{k}) \]

- High T_c d-wave superconductivity tested by phase sensitive Josephson junction experiment by Van Harlingen et al.
Unconventional BEC: beyond “no-node”

• The condensate wavefunction $\Psi(r)$ belongs to a non-trivial (non-s-wave) representation of the lattice point group.

• No-node theorem does NOT apply to excited states.

• Example: the p-orbital bands can have degenerate band minima.

Interaction selects complex $p+ip$ UBEC:

$$\Psi(\vec{r}) = \Psi_{K_1}(\vec{r}) + i\Psi_{K_2}(\vec{r})$$

• Solid state experiments: d-wave BEC in exiton-polariton lattices (Kim, Yamamoto, Wu)

• Real numbers $\rightarrow$ complex numbers $\rightarrow$ quaternions (Q).

• Bosons: real (positive) BEC $\rightarrow$ complex BEC $\rightarrow$ Q-BEC unconventional symm. beyond the “no-node” theorem. p-wave BEC, and topological spin textures

• Fermions: Q-analytic Landau levels in 3D.

  harmonic potential+ spin-orbit coupling Cauchy-Riemann-Fueter condition.

• Complex quaternions: 3D Landau levels of Dirac fermions.
Two-component spinor $\rightarrow$ quaternion

• A quaternion can also be understood as a pair of complex numbers just like complex number is a pair of real numbers.

• Spinor wavefunction $\rightarrow$ quaternion wavefunction; Spin density distribution $\rightarrow$ 1st Hopf-mapping.

\[
\psi(r, \hat{\Omega}) = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}
\]

\[
\xi(r, \hat{\Omega}) = \text{Re} \psi_\uparrow + \text{Im} \psi_\downarrow i - \text{Re} \psi_\downarrow j + \text{Im} \psi_\uparrow k
\]

\[
\vec{S}(r, \hat{\Omega}) = \psi^+(r, \hat{\Omega}) \frac{\vec{\sigma}}{2} \psi^+(r, \hat{\Omega})
\]

\[
S_x i + S_y j + S_z k = \frac{1}{2} \xi k \xi
\]
The 2D version: BEC with Rashba SO coupling

- Solid state SO coupled boson system: excitons in semiconductors.

- Free space: Spin spiral stripe for density-only interactions. (“order from disorder” mechanism beyond G-P level.)

  Trap: Prediction of spontaneous generation of “baby” skyrmion spin-texture and half-quantum vortex.

- Spin-textures in SO coupled exciton condensates observed from photoluminescence by L. Butov.
3D SO coupling in hyperfine states of $^{40}$K atoms

$$H^{3D} = -\frac{\hbar^2 \nabla^2}{2m} + \frac{1}{2} m \omega^2 r^2 - \lambda (-i\hbar \nabla \cdot \sigma)$$

Artificial SO coupling from light-atom interaction

Yi Li, Xiangfa Zhou, C. Wu, PRB 85, 125122 (2012).
Spherical rotator subjected to a fundamental monople

\[ H = -\frac{\hbar^2 \nabla^2}{2m} + \lambda (-i\hbar \bar{\nabla} \cdot \vec{\sigma}_{\alpha\beta}) + \frac{1}{2} m \omega_T^2 r^2 \]

- Low energy SO sphere with radius \( k_{so} \).
  Dimensionless SO coupling strength

\[ \hbar k_{so} = m\lambda, \quad l_T = \sqrt{\frac{\hbar}{m\omega}}, \quad \alpha = k_{so} l_T \]

- Momentum space:

\[ V_{ex}(r) = \frac{1}{2} M \omega_T^2 r^2 \rightarrow \frac{1}{2} M \omega_T^2 \left( i\nabla_k - A(k) \right)^2, \]

\[ \iiint d^2k \nabla \times A_k = 2\pi \]

- Angular momentum quantization change to half-integer values.
TR invariant parity breaking 3D Landau-levels

• Angular dispersion suppressed by strong SO coupling forming nearly flat Landau levels.

\[ E_{n_r,j_z} \approx \frac{j(j + 1)}{2\alpha^2} \hbar \omega_r + (n_r + \frac{1}{2}) \hbar \omega_r \]

\[ n_r = 1 \]
\[ n_r = 0 \]

• LLL wavefunctions through SO coupled harmonics:

\[
\psi_{3D,jj_z}(\vec{r}) = e^{-\frac{\alpha^2}{2l_r^2}} \left\{ j_l(k_0 r) Y_{+,j,l,j_z}(\Omega_r) + i j_{l+1}(k_0 r) Y_{-,j,l+1,j_z}(\Omega_r) \right\},
\]

Yi Li, Xiangfa Zhou, C. Wu, PRB 85, 125122 (2012); Gosh et al, PRA 84, 053629 (2011).
The single-particle ground state (mixed s and p-partial wave)

\[ \psi_{j=j_z=\frac{1}{2}}(r, \hat{\Omega}) = e^{-\frac{r^2}{2l^2}} (j_0(k_{so} r) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + ij_1(k_{so} r) \begin{pmatrix} \cos \theta \\ \sin \theta e^{i\phi} \end{pmatrix}) \]

- Quaternion representation:

\[ \xi(r, \hat{\Omega}) = \text{Re} \psi_\uparrow + \text{Im} \psi_\downarrow i - \text{Re} \psi_\downarrow j + \text{Im} \psi_\uparrow k \]

\[ = | \xi(r) | e^{\omega(\hat{\Omega})\gamma(r)} \]

\[ = | \xi(r) | (\cos \gamma + \omega(\hat{\Omega}) \sin \gamma) \]

- Imaginary unit \( \leftrightarrow \) solid angle direction

\[ \omega(\hat{\Omega}) = i \sin \theta \cos \phi + j \sin \theta \sin \phi + k \cos \theta \]
BEC WF as a quaternionic defect

- Condensation WF based on single-particle GS.

\[ \xi(r, \Omega) = |\xi(r)| (\cos \gamma + \omega(\Omega) \sin \gamma) \]

\[ \tan \gamma(r) = \frac{g}{f} \]

\[ \omega(\Omega) = i \sin \theta \cos \phi + j \sin \theta \sin \phi + k \cos \theta \]

- Along any \( \Omega \), \( e^{\omega(\Omega) \gamma(r)} \) winds in \((1, \omega(\Omega))-plane\) as \( r \) increases. \( \gamma(r_n) = n\pi \) at zero points of \( g(r) \).

- Mapping from 3D real space to quaternionic phase space \( S^3 \) – 3D skrymion.
Quaternionic defect with non-zero Hopf invariant

- 3D spin distribution: the horizontal cross-section \( z=0 \) is a baby (2D) skrymion.

\[
\begin{align*}
\begin{bmatrix} S_x(r) \\ S_y(r) \end{bmatrix} &= \xi^2(r) \sin \gamma \sin \theta \begin{bmatrix} \cos \phi, -\sin \phi \\ \sin \phi, \cos \phi \end{bmatrix} \begin{bmatrix} \sin \gamma \cos \theta \\ \cos \gamma \end{bmatrix} \\
S_z(r) &= \xi^2(r) (\cos^2 \gamma + \sin^2 \gamma \cos 2\theta)
\end{align*}
\]

\[\pi_3(S^2) = Z\]

xy-plane \( z/l_r = 0.5 \)

\[\alpha = 1.5, \ c = 1, \ \text{and} \ \beta = 30,\]
See the linking number

• The trajectory of spin with the same orientation form a closed loop (in our case, the loop may be cut by the boundary).

• For \( \vec{S} /\!/ \hat{z} \), \( \theta = 0, \pi \); reduced to a straight line of the \( z \)-axis

For \( \vec{S} /\!/ -\hat{z} \), \( \theta = \frac{\pi}{2}, \gamma = \frac{\pi}{2} \); a circle in the equatorial plane

\[
S_z(r) = \xi^2(r) (\cos^2 \gamma + \sin^2 \gamma \cos 2\theta)
\]

• For any two loops, they link each other.
3D quaternion analogy to 2D Abrikosov vortex lattice

- As SO coupling goes strong, the condensate WF mixes different single particle states within the same LL driven by interaction.
- Rotational symmetry is broken forming texture lattices.

\[ \alpha = 15, \beta = 0.8, c = 1 \]
• Real numbers $\rightarrow$ complex numbers $\rightarrow$ quaternions.

• **Positive BEC** $\rightarrow$ **complex BEC** $\rightarrow$ **quaternionic BEC**

  go beyond the “no-node” theorem

  p-wave BEC, and topological spin textures

• Quaternionic analytic Landau levels in 3D.

  harmonic potential + spin-orbit coupling
  Cauchy-Riemann-Fueter condition.

• Complex quaternions: 3D Landau levels of Dirac fermions.
3D quaternionic (SU(2)) Landau levels

2D LLs (continuum, flat spectra and complex analyticity); IQHE & FQHE.

QM: (Final exam for grad students.) harmonic oscillator + spin-orbit coupling (symm-like gauge) degenerate helical modes; math: quaternionic analyticity

3D TI (lattice) Frac-TI (3D Laughlin WF)?

Exp. realization: cold atom; semiconductors?

Dirac fermion: flat band of zero modes from non-minimal coupling; novel anomaly?

H^{3D \text{Dirac LL}}_{\text{symm}} = \frac{\hbar \omega}{2} \begin{pmatrix} 0 & i\vec{\sigma} \cdot \vec{a}^+ \\ -i\vec{\sigma} \cdot \vec{a} & 0 \end{pmatrix}
Return to Landau levels (a review of 2D)

• **Simple, explicit and elegant.**

Symmetric gauge: analytic functions of complex variables (chiral).

\[
\psi_{LLL}^{\text{sym}} = z^m e^{-|z|^2/(2l_B^2)}, \quad z = x + iy, \quad m \geq 0.
\]

Landau gauge: 1D harmonic oscillators with center-shift (k_x dep.) spatial separation of chiral modes.

\[
\psi_{LLL}^{\text{Landau}} = e^{-(y - y_0(k_x))^2/(2l_B^2)} e^{ik_x x}
\]

\[
y_0 = l_B^2 k_x
\]
Comparison of symm gauge LLs in 2D and 3D

• 1D harmonic levels: real polynomials.

• 2D LLs: complex analytic polynomials.

\[ \psi_{LLL}^{\text{sym}} = z^m e^{-|z|^2/(2l_h^2)} , \quad z = x + iy , \quad m \geq 0. \]

• 3D LLs: SU(2) group space \( \rightarrow \) quaternionic analytic polynomials.

\[ \psi_{j_+, \text{ high}}^{LLL} (r, \Omega) = [(\hat{e}_1 + i\hat{e}_2) \cdot \vec{r}]^l \otimes \chi_{\hat{e}_3} e^{-r^2/2l_g^2} \]
Conclusions

• Quaternion is a beautiful and useful concept.

• The 3D spin-orbit coupled BEC exhibit the 3D structure of quaternionic defects with non-zero Hopf invariants.

• Landau levels are generalized to 3D with the full rotational symmetry and TR symmetry.

• Quaternionic analyticity is a useful criterion to select good 3D wavefunctions for non-trivial topology.

Proposal: Quantum Mechanics class instruction (Final or qual exams).
Landau-level (LL) type single particle quantization (2D)

- The Rashba ring in momentum space with the radius $k_{so}$. Dimensionless SO coupling strength $\alpha$.

$$l_T = \sqrt{\frac{\hbar}{m \omega_T}}, \quad \alpha = k_{so} l_T \gg 1$$

- Ring rotor in momentum space subjected to a $\pi$–flux $\rightarrow$ half integer quantized angular momentum.

$$V_{ex}(r) = \frac{1}{2} M \omega_T^2 r^2 \rightarrow \frac{1}{2} M \omega_T^2 \left( i \nabla_k - A(k) \right)^2, \quad \oint A(k) dk = \pi$$

- Angular dispersion is suppressed by strong SO coupling forming nearly flat Landau levels.

$$E_{n_r,j_z} = n_r \hbar \omega_T + \frac{j_z^2}{2\alpha^2} \hbar \omega_T + \text{const}$$

SO coupled bosons in trap: spin textures and half-quantum vortex

- Weak SO coupling. Condensate WFs:

\[ |\psi_{1/2} \rangle = \begin{pmatrix} f(r) \\ g(r)e^{i\phi} \end{pmatrix}, \quad j_z = L + S = 1/2 \]

- Friedel-like oscillation of \( |f(r)|^2 \) (up), and \( |g(r)|^2 \) (down) at the pitch value of \( k_{so} \).

- The relative phase shift \( \frac{\pi}{2} \) between \( f(r) \) and \( g(r) \).

- 2D (baby) skyrmion type spin texture formation and half-quantum vortex.

\[ \langle S_z \rangle = |f|^2 - |g|^2, \quad \langle S_x \rangle = fg \cos \phi, \quad \langle S_y \rangle = fg \sin \phi \]
Spin lines with non-zero Hopf invariant

- 3D spin configuration with non-trivial Hopf-invariant; twisted baby (2D) skrymion as moving along z-axis.