

Geometric theory of quantum spin systems

Patrick Bruno, *ESRF Theory Group*

Summary

- Introduction: classical magnets vs. quantum magnets
- Majorana's stellar representation of quantum spin states
- spin wavefunction as a (fictitious) thermodynamics partition function
- Berry's geometric phase in Majorana representation
- Towards a geometric theory of quantum many-spin systems

Introduction: *Classical magnets vs. quantum magnets*

classical concept for a magnet:

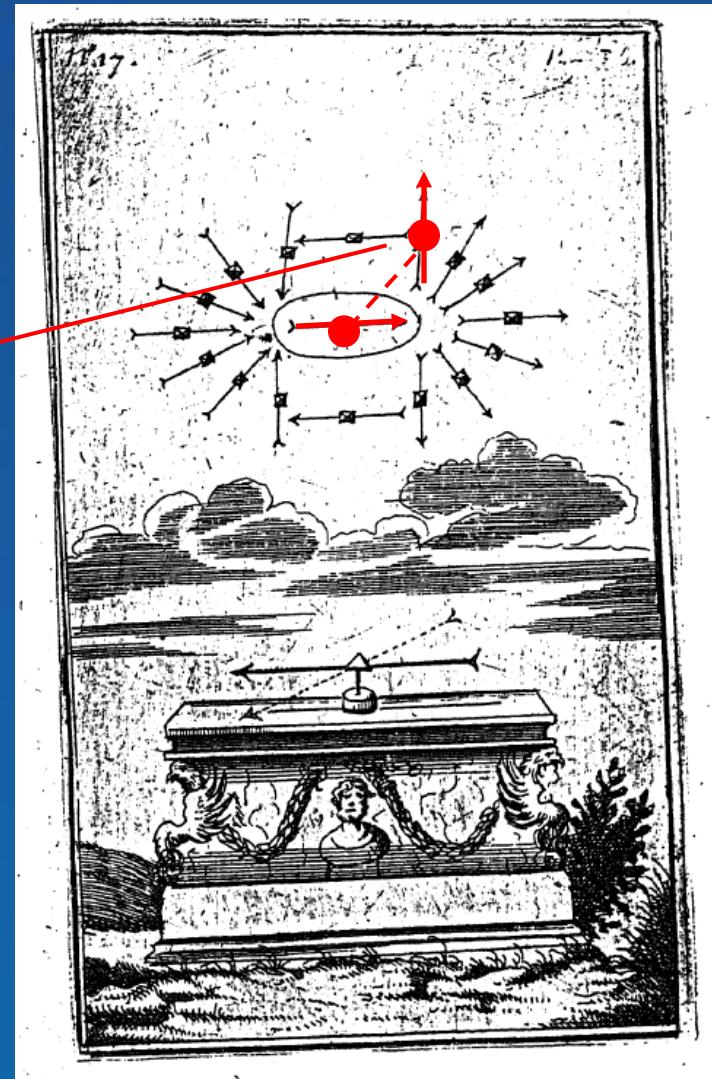
Petrus Peregrinus de Maricourt (13th cent.), William Gilbert (16th cent.)



object with the
property of being
able to point into
a certain direction
(= dipole moment)

dynamics of a
magnet = changes
of its orientation

"Traité de l'aiman"
Dalencé (1691)





$$\mathbf{m} = m \mathbf{u}$$

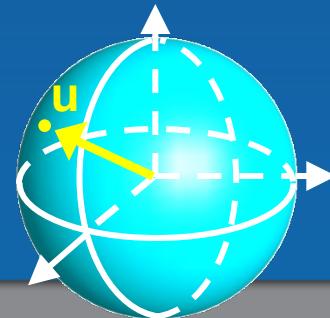
$$m = \text{constant}$$

dynamics described by
classical equations
(Landau-Lifshitz-Gilbert)

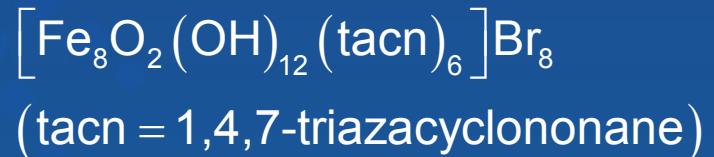
$$m \frac{d\mathbf{u}}{dt} = \gamma \mathbf{B}_{\text{eff}} \times \mathbf{u} + \text{damping term}$$

$$\mathbf{B}_{\text{eff}} = -\frac{1}{m} \frac{dE}{d\mathbf{u}}$$

= equation of motion
of a *classical* gyroscope
= dynamics of a point on a
sphere
(phase space of dimension 2)



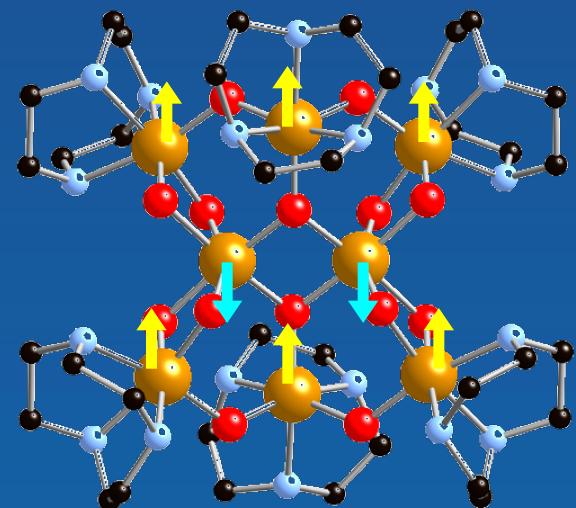
molecular magnets



Fe_8

$$\begin{array}{l} \text{6 ions } \text{Fe}^{3+} \quad S = 5/2 \quad (\uparrow) \\ \text{2 ions } \text{Fe}^{3+} \quad S = 5/2 \quad (\downarrow) \end{array} \quad \left. \right\} \Rightarrow S = 10$$

$$\hat{\mathcal{H}} = -\mathbf{H} \cdot \mathbf{S} - K S_z^2 + D(S_x^2 - S_y^2)$$



genuine quantum effects:

tunneling, quantum interferences, entanglement ...

Quantum spin systems with exotic ordering

spin nematics (magnets without dipole moments)

Example:

spin $S=1$

$$\left. \begin{array}{l} |1,1\rangle = \uparrow \\ |1,-1\rangle = \downarrow \\ |1,0\rangle = \uparrow\downarrow \end{array} \right\} \begin{array}{l} \mathbf{m} \neq 0 \quad (\text{dipole moment}) \\ \mathbf{m} = 0, \quad Q_{zz} \neq 0 \quad (\text{quadrupole moment}) \end{array}$$

$$H = - \sum_{<i,j>} \left[J_1 (\mathbf{S}_1 \cdot \mathbf{S}_2) + J_2 (\mathbf{S}_1 \cdot \mathbf{S}_2)^2 \right] \quad 0 < J_1 < J_2$$

→ spontaneous quadrupolar ordering

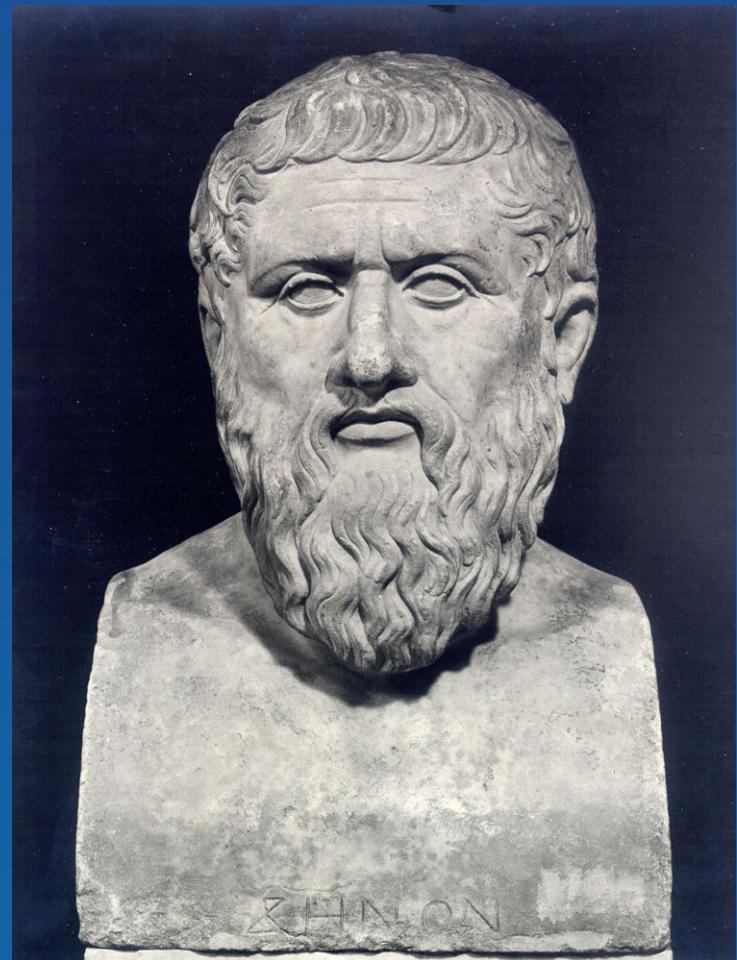
cf. ultracold spin 1 gases

cf. “hidden” order in heavy-fermions systems
(hexadecapole ordering, or even higher multipolar ordering, has been proposed)

Majorana's stellar representation of quantum spin states

ΑΓΕΩΜΕΤΡΗΤΟΣ
ΜΗΔΕΙΣ ΕΙΣΙΤΩ
(ΠΛΑΤΩΝ)

**"Let no one ignorant of
geometry enter here"**
(inscription above the entrance
of Plato's Academy in Athens)



Plato (427-347 B.C.)

traditional description of spin systems

quantum state: $|\psi\rangle$

select some axis z

basis set = eigenstates of J_z :

$|JM\rangle$ ($M = J, J-1, J-2, \dots, -J$)

$$\psi(M) = \langle JM | \psi \rangle$$

matrix element of the Hamiltonian:

$$H_{MM'} = \langle JM | \hat{H} | JM' \rangle$$

- convenient for numerical calculations
- physically not very insightful (except for particular cases)
- needs to single out some arbitrary axis

spin coherent states

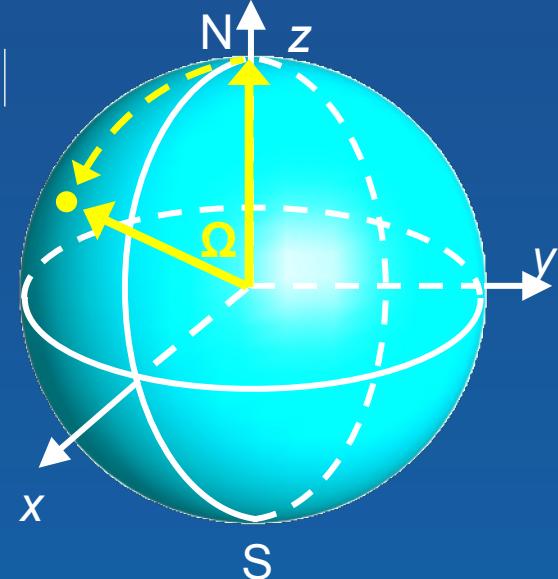
$|\underline{\Omega}\rangle = (|JJ\rangle \text{ rotated to the } \underline{\Omega} \text{ axis})$

$$1 = \frac{2J+1}{4\pi} \int d\underline{\Omega} |\underline{\Omega}\rangle \langle \underline{\Omega}|$$

$$\psi(\underline{\Omega}) = \langle \underline{\Omega} | \psi \rangle$$

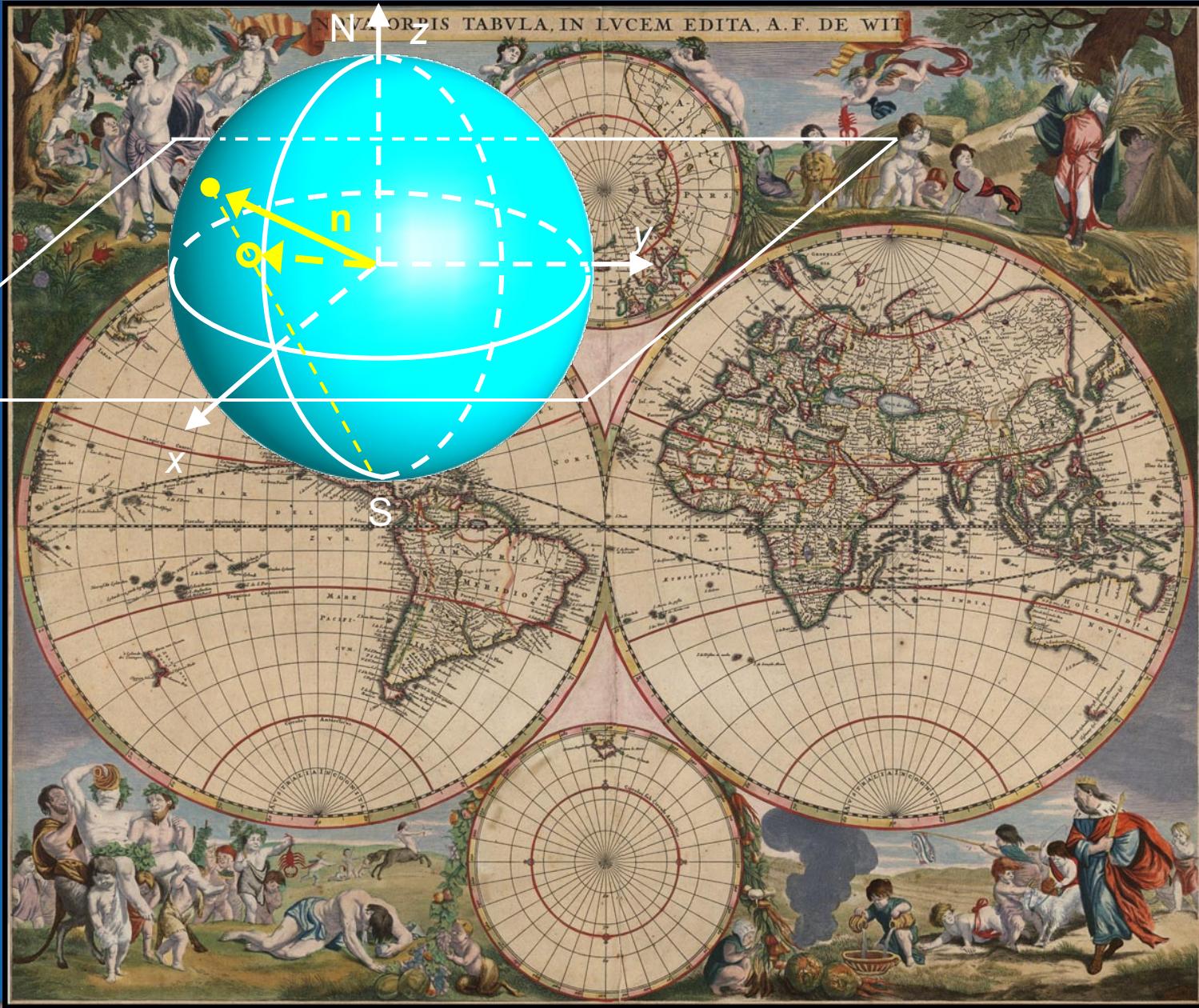
$$Q_\psi(\underline{\Omega}) = |\psi(\underline{\Omega})|^2$$

$$H(\underline{\Omega}) = \langle \underline{\Omega} | \hat{H} | \underline{\Omega} \rangle$$



- “geometrically” more satisfactory description (no need to single out some axis)
- the quantum state is entirely characterized by the so-called Husimi function $Q_\psi(\underline{\Omega}) = |\psi(\underline{\Omega})|^2$
- the Hamiltonian is entirely described by its *diagonal* matrix elements $H(\underline{\Omega}) = \langle \underline{\Omega} | \hat{H} | \underline{\Omega} \rangle$

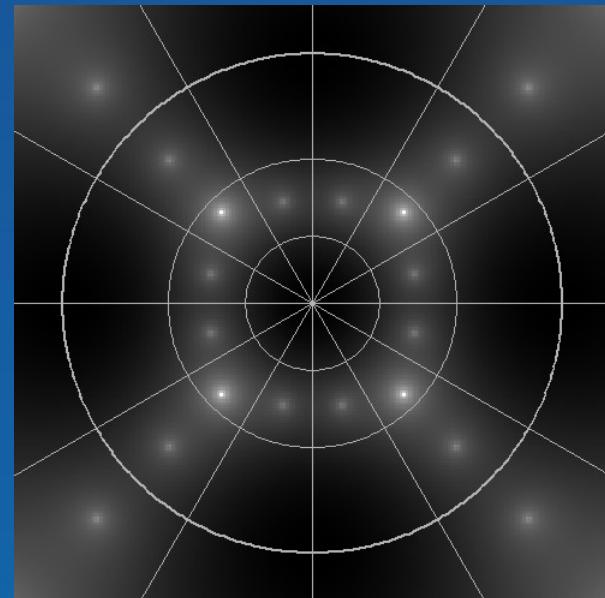
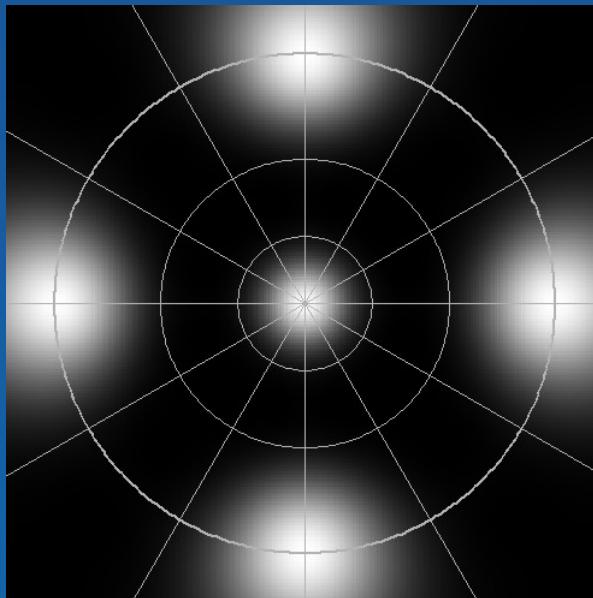
stereographic projection



cubic anisotropy
(ground state)

$S = 20$

$$H = \frac{-3K}{S^2(S+1)^2} (S_x^4 + S_y^4 + S_z^4)$$



$$Q_\psi(\mathbf{n}) = |\psi(\mathbf{n})|^2$$

$$\text{Log}\left(\frac{1}{Q_\psi(\mathbf{n})}\right)$$

Majorana's "stellar" representation

the wave function $\psi(\Omega) = \langle \underline{\Omega} | \psi \rangle$ or the Husimi distribution $Q_\psi(\Omega) = |\psi(\Omega)|^2$ of a system with spin J has *exactly* $2J$ zeros (= **stars**)

the quantum state $|\psi\rangle$ is entirely characterized by the location of its $2J$ stars (= **constellation**)

for a coherent state $|\underline{\Omega}\rangle$, the Majorana stars are all degenerate and located at the antipode of Ω

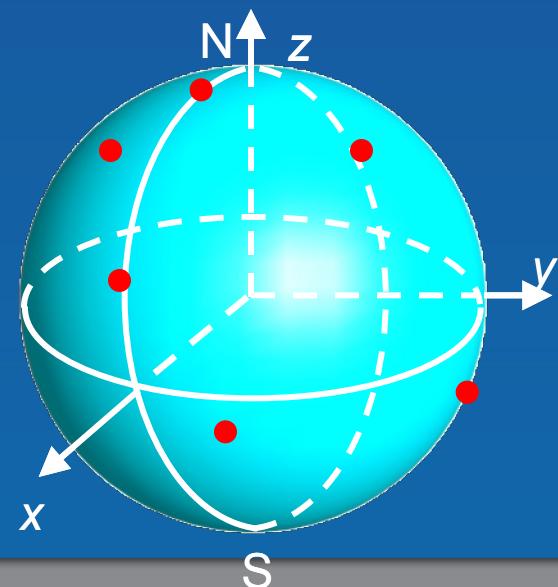
coherent are *quasi-classical* states
(smallest transverse spread)

entangled (non-classical) states are characterized by Majorana stars that are *not all degenerate*

↔ a generic spin J state is obtained as a *unique* fully symmetrized product of $2J$ spin $\frac{1}{2}$ states



Ettore Majorana
(1906 – 1938 (?))



spin wavefunction as a (fictitious)
thermodynamics partition function

spin $\frac{1}{2}$ coherent state: $|\underline{\Omega}\rangle = \cos\left(\frac{\theta}{2}\right)|\hat{\mathbf{z}}\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|-\hat{\mathbf{z}}\rangle$

scalar product of 2 spin 1/2 states: $\langle \underline{\Omega}_1 | \underline{\Omega}_2 \rangle = \left(\frac{1 + \underline{\Omega}_1 \cdot \underline{\Omega}_2}{2} \right)^{1/2} \exp\left(i \frac{\Sigma(\hat{\mathbf{z}}, \underline{\Omega}_1, \underline{\Omega}_2)}{2}\right)$
 $\Sigma(\hat{\mathbf{z}}, \underline{\Omega}_1, \underline{\Omega}_2) = \text{oriented area of spherical triangle } (\hat{\mathbf{z}}, \underline{\Omega}_1, \underline{\Omega}_2)$

spin J coherent state: $|\underline{\Omega}\rangle \equiv \underbrace{|\underline{\Omega}\rangle \otimes |\underline{\Omega}\rangle \otimes \dots \otimes |\underline{\Omega}\rangle}_{2J \text{ factors}} \equiv |\underline{\Omega}\rangle^{\otimes(2J)}$

(unnormalized) spin $2J$ state parametrized

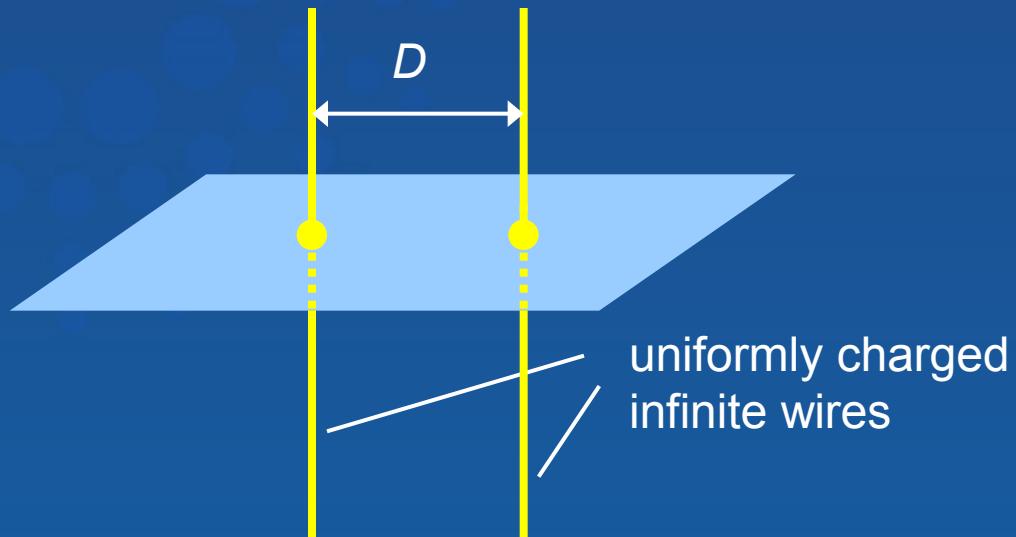
by its $2J$ Majorana stars $\{\mathbf{n}_i\}$ ($i = 1, \dots, 2J$): $|\tilde{\Psi}\{\mathbf{n}_i\}\rangle \equiv \frac{1}{(2J)!} \sum_{P \in \text{perms}(2J)} \left[\bigotimes_{i=1}^{2J} |-\mathbf{n}_{P(i)}\rangle \right]$

norm of state $|\tilde{\Psi}\rangle$: $Z_J(\tilde{\Psi}) \equiv \langle \tilde{\Psi} | \tilde{\Psi} \rangle = \frac{2J+1}{4\pi} \int d^2\Omega \langle \tilde{\Psi} | \underline{\Omega} \rangle \langle \underline{\Omega} | \tilde{\Psi} \rangle$

 $= \frac{2J+1}{4\pi} \int d^2\Omega \left[\prod_{i=1}^{2J} \left(\frac{1 - \underline{\Omega} \cdot \mathbf{n}_i}{2} \right) \right]$

planar 2D Coulomb interaction

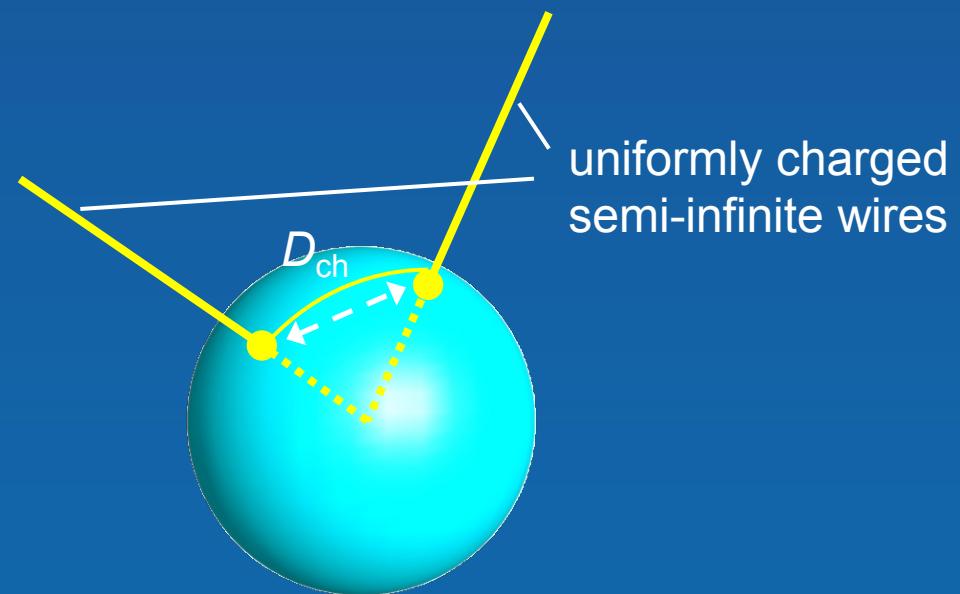
$$U_{\text{2D-pl}} \propto -q_1 q_2 \ln(D) + C$$



spherical 2D Coulomb interaction

$$U_{\text{2D-sph}} \propto -q_1 q_2 \ln(D_{\text{ch}}) + C$$

$$\text{chordal distance: } D_{\text{ch}} = 2 \sin\left(\frac{\theta}{2}\right)$$



probability of finding our system in the coherent state $|\underline{\Omega}\rangle$:

$$P_{\tilde{\Psi}}(\underline{\Omega}) \equiv \frac{(2J+1)}{Z_J(\tilde{\Psi})} |\langle \tilde{\Psi} | \underline{\Omega} \rangle|^2 = \frac{(2J+1)}{Z_J(\tilde{\Psi})} \prod_{i=1}^{2J} \sin^2\left(\frac{\theta_{\underline{\Omega}, \mathbf{n}_i}}{2}\right)$$

$$= \frac{(2J+1)}{Z_J(\tilde{\Psi})} \exp(-\beta V_{\tilde{\Psi}}(\underline{\Omega}))$$

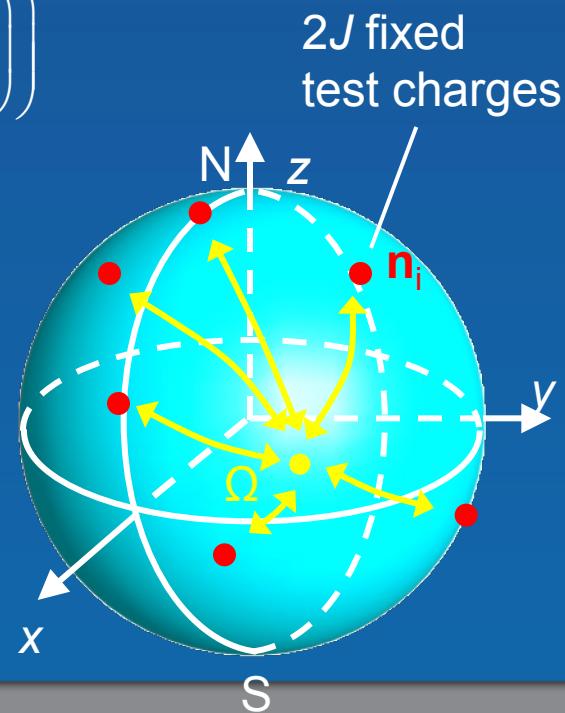
with inverse "temperature" $\beta = 1$ and $V_{\tilde{\Psi}}(\underline{\Omega}) \equiv \sum_{i=1}^{2J} V(\underline{\Omega}, \mathbf{n}_i)$

spherical "Coulomb repulsion" : $V(\underline{\Omega}, \mathbf{n}_i) \equiv -\ln\left(2 \sin\left(\frac{\theta_{\underline{\Omega}, \mathbf{n}_i}}{2}\right)\right)$

$$Z_J(\tilde{\Psi}) = \frac{2J+1}{4\pi} \int d^2\underline{\Omega} \exp(-\beta V_{\tilde{\Psi}}(\underline{\Omega}))$$

= partition function of a fictitious gas
of independent particles interacting
with $2J$ fixed test charges

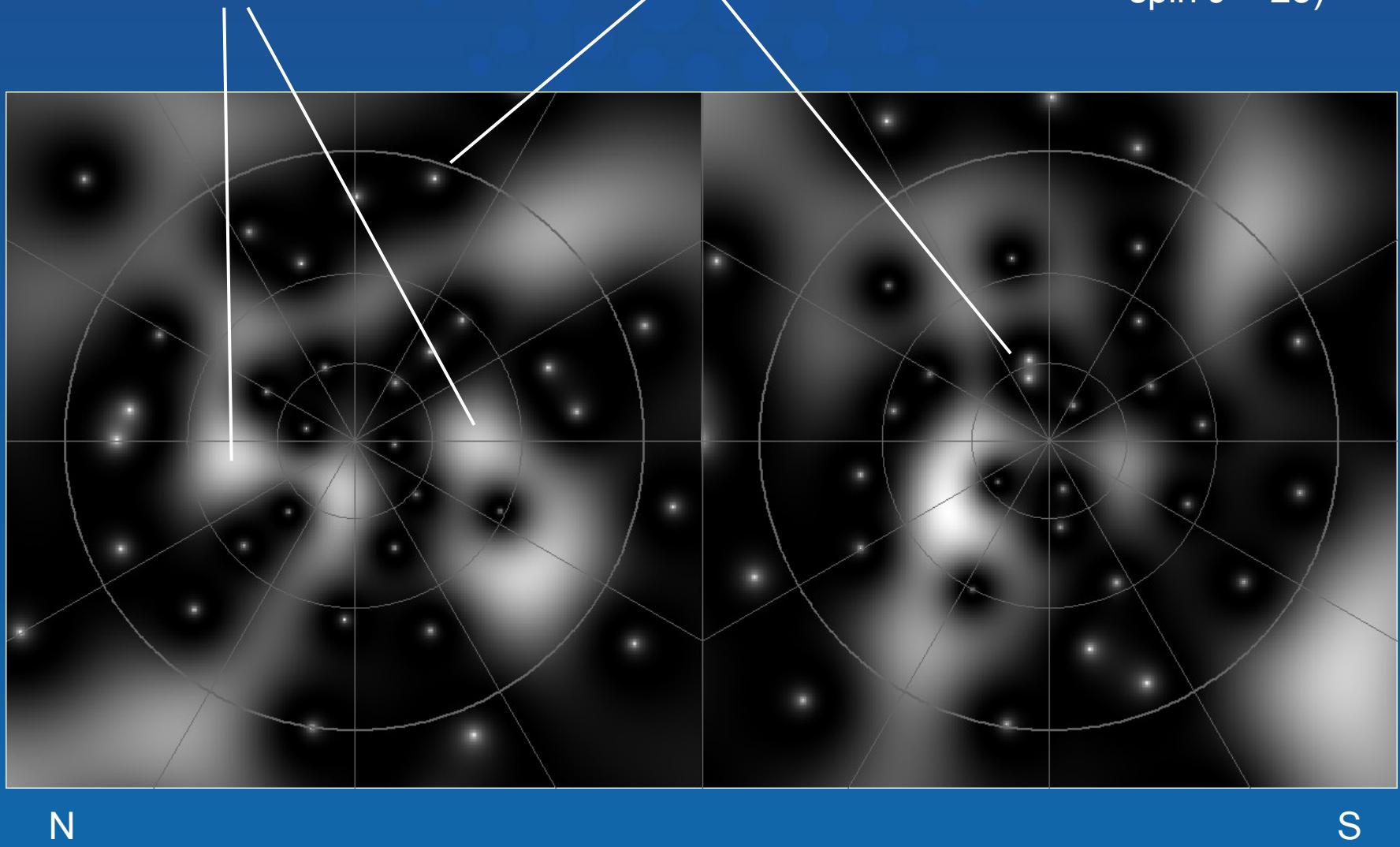
fictitious free energy: $F(\tilde{\Psi}) \equiv -\frac{1}{\beta} \ln(Z_J(\tilde{\Psi}))$



probability density
= fictitious gas density

Majorana stars

(random state of
spin $J = 25$)



N

S

from known expressions of Z_J one can derive explicit expressions for the expectation value of the dipole moment for arbitrary value of J :

$$\langle \mathbf{J} \rangle = -\frac{1}{2} \mathbf{n}_1 \quad (J=1/2)$$

$$\sigma_{ij} \equiv \sin^2\left(\frac{\theta_{ij}}{2}\right) = \frac{1 - \mathbf{n}_i \cdot \mathbf{n}_j}{2}$$

$$\langle \mathbf{J} \rangle = -\frac{1}{2} \frac{\mathbf{n}_1 + \mathbf{n}_2}{1 - \frac{\sigma_{12}}{2}} \quad (J=1)$$

$$\langle \mathbf{J} \rangle = -\frac{1}{2} \frac{\mathbf{n}_1 \left(1 - \frac{\sigma_{23}}{3}\right) + \mathbf{n}_2 \left(1 - \frac{\sigma_{13}}{3}\right) + \mathbf{n}_3 \left(1 - \frac{\sigma_{12}}{3}\right)}{1 - \frac{\sigma_{12} + \sigma_{13} + \sigma_{23}}{3}} \quad (J=3/2)$$

etc...

+ expressions of higher multipoles (quadrupole, octupole, etc...)
(systematic diagram technique)

→ expression of the (real !) energy in terms of the Majorana stars: $H(\tilde{\Psi}) \equiv \frac{\langle \tilde{\Psi} | \hat{H} | \tilde{\Psi} \rangle}{\langle \tilde{\Psi} | \tilde{\Psi} \rangle}$

e.g.: $H(\tilde{\Psi}) = -\mathbf{B} \cdot \langle \mathbf{J} \rangle + K \langle J_z^2 \rangle + D \left(\langle J_x^2 \rangle - \langle J_y^2 \rangle \right) + \dots = H\{\mathbf{n}_i\}$

quantum metric

the fictitious free-energy determines the quantum metric:

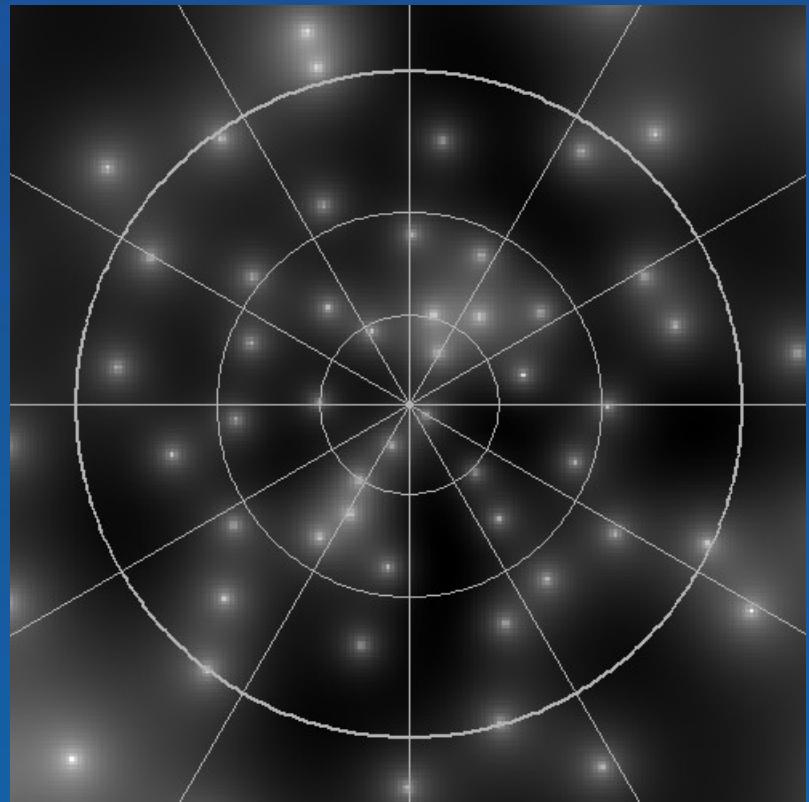
$$\bar{\mathbf{g}}_{ij} = \frac{\partial^2 F(\tilde{\Psi})}{\partial \mathbf{n}_i \partial \mathbf{n}_j}$$

allows to measure the quantum (so-called Fubini-Study) distance between quantum states

the metric becomes degenerate, i.e., the volume measure $\sqrt{\det(\bar{\mathbf{g}})}$ goes to zero, whenever two or more Majorana stars coincide

- statistical (Coulomb) repulsion of Majorana stars
- = consequence of the bosonic character of the Majorana stars

$J = 40$ stereographic representation



random Hamiltonian

(classically chaotic system)
Leboeuf *et al.* (1990); Hannay (1996)

Berry's geometric phase in Majorana representation

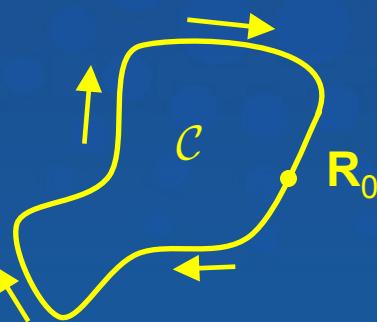
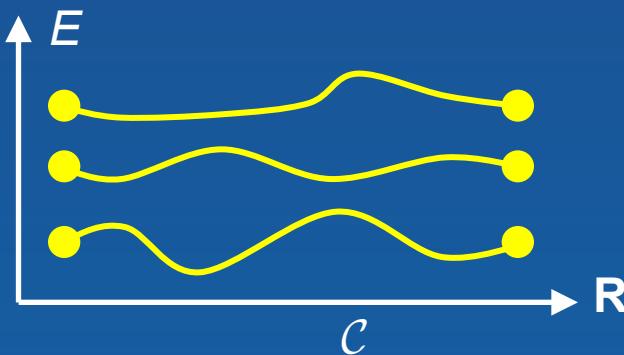
Berry phase in a nutshell

M.V. Berry,
Proc. Roy. Soc. London A **392**, 45 (1984)

Hamiltonian: $\hat{\mathcal{H}}(\mathbf{R})$



set of external parameters



what is the value
of this phase ???

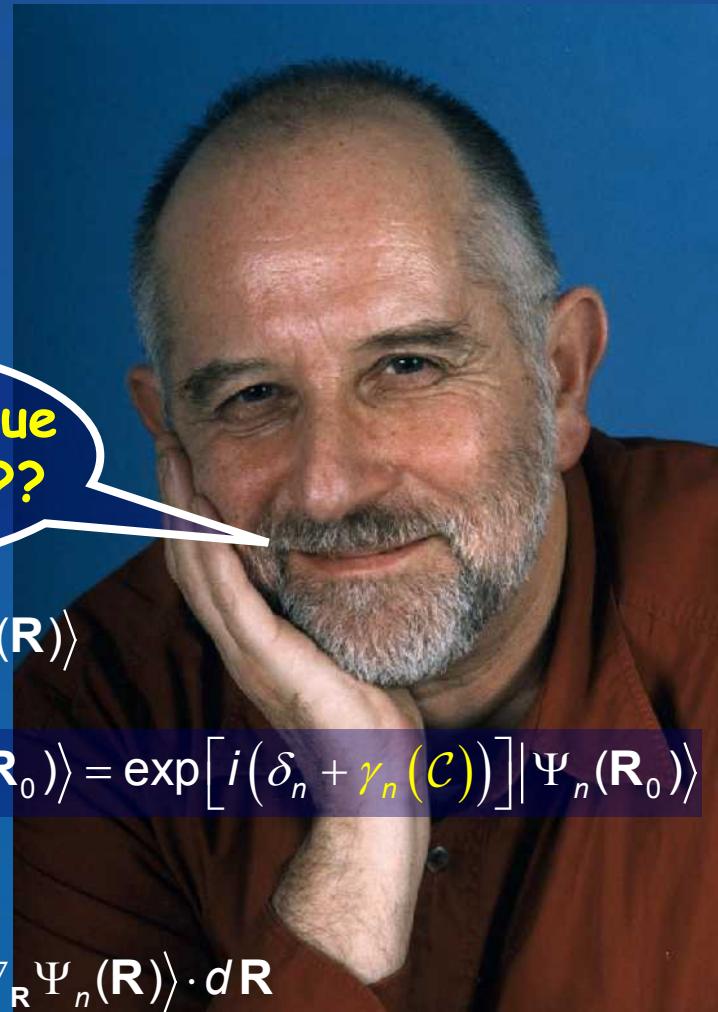
basis states: $|\Psi_n(\mathbf{R})\rangle$

$$\hat{\mathcal{H}}(\mathbf{R})|\Psi_n(\mathbf{R})\rangle = E_n(\mathbf{R})|\Psi_n(\mathbf{R})\rangle$$

adiabatic transformation: $|\Psi_n(\mathbf{R}_0)\rangle \xrightarrow{C} |\Psi'_n(\mathbf{R}_0)\rangle = \exp[i(\delta_n + \gamma_n(C))]\Psi_n(\mathbf{R}_0)\rangle$

δ_n = dynamical phase

non-integrable (Berry) phase: $\gamma_n(C) = i \oint_C \langle \Psi_n(\mathbf{R}) | \nabla_{\mathbf{R}} \Psi_n(\mathbf{R}) \rangle \cdot d\mathbf{R}$



Sir Michael V. Berry

Berry phase as a fictitious flux in parameter space (3D)

geometric (Berry) phase: $\gamma_n(\mathcal{C}) = i \oint_{\mathcal{C}} \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle \cdot d\mathbf{R}$

$$= \oint_{\mathcal{C}} \mathbf{A}^n(\mathbf{R}) \cdot d\mathbf{R}$$

with $\mathbf{A}^n(\mathbf{R}) = i \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle$ (Berry connection)

Stokes' theorem: $\gamma_n(\mathcal{C}) = \iint_S \mathbf{B}^n(\mathbf{R}) \cdot \mathbf{n} dS$ (\mathbf{B}^n = Berry curvature)

with $\mathbf{B}^n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}(\mathbf{R})$

$$= i \langle \nabla_{\mathbf{R}} n | \times | \nabla_{\mathbf{R}} n \rangle$$

$$= i \sum_{m(\neq n)} \langle \nabla_{\mathbf{R}} n | m \rangle \times \langle m | \nabla_{\mathbf{R}} n \rangle$$



$$\mathbf{B}^n(\mathbf{R}) = i \sum_{m(\neq n)} \frac{\langle n | \nabla_{\mathbf{R}} \hat{\mathcal{H}} | m \rangle \times \langle m | \nabla_{\mathbf{R}} \hat{\mathcal{H}} | n \rangle}{(E_m(\mathbf{R}) - E_n(\mathbf{R}))^2}$$

$\mathbf{B}^n(\mathbf{R})$ is large if \mathbf{R} is close to a degeneracy \mathbf{R}^*
(flux of a Dirac monopole located at \mathbf{R}^*)

Canonical example of Berry phase: spin in a magnetic field

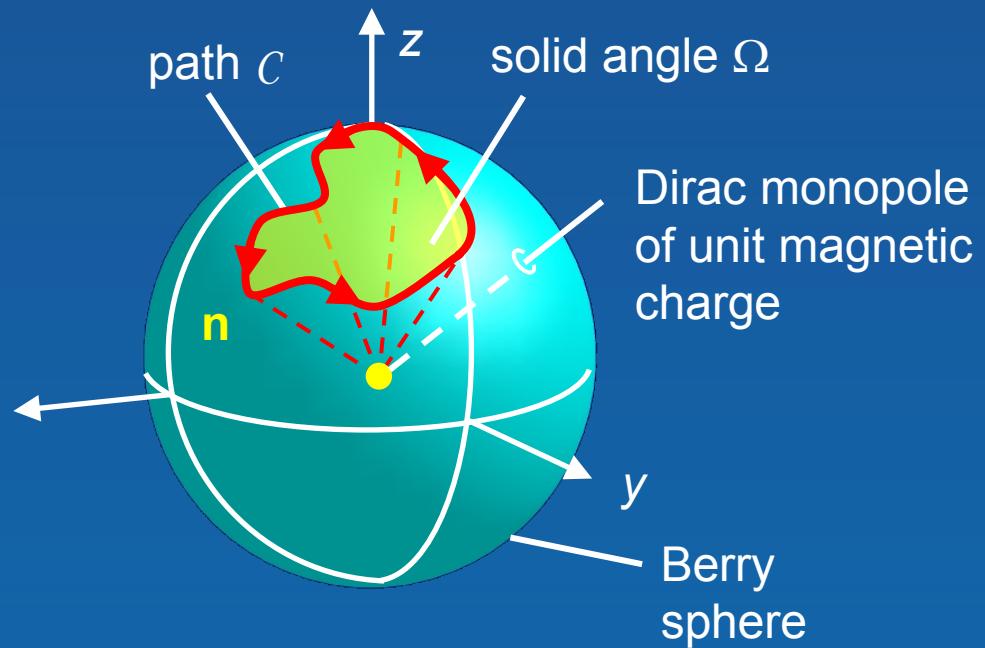
Hamiltonian: $\hat{\mathcal{H}}(\mathbf{n}) = -\mathbf{B} \cdot \mathbf{J} = -B \mathbf{n} \cdot \mathbf{J}$

external parameter = unit vector \mathbf{n}

Berry phase: $\gamma_c = -M \Omega$

$$M = J, J-1, \dots, -J$$

= Aharonov-Bohm phase of an electric charge $2M$ in the magnetic field of a Dirac monopole of unit magnetic charge



quantization of the Dirac monopole \leftrightarrow topology

Berry connection (= “vector potential”):

$$A_\alpha \equiv \frac{i}{2} \left[\frac{\langle \tilde{\Psi} | \partial_\alpha \tilde{\Psi} \rangle - \langle \partial_\alpha \tilde{\Psi} | \tilde{\Psi} \rangle}{\langle \tilde{\Psi} | \tilde{\Psi} \rangle} \right]$$

Berry curvature (= “flux” density): $f_{\alpha\beta} \equiv \partial_\alpha A_\beta - \partial_\beta A_\alpha$

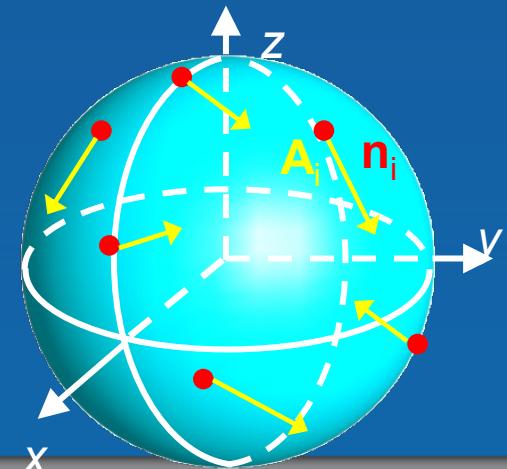
$$f_{\alpha\beta} = \frac{i}{2} \left[\frac{\langle \partial_\alpha \tilde{\Psi} | \partial_\beta \tilde{\Psi} \rangle - \langle \partial_\beta \tilde{\Psi} | \partial_\alpha \tilde{\Psi} \rangle}{\langle \tilde{\Psi} | \tilde{\Psi} \rangle} - \frac{\langle \partial_\alpha \tilde{\Psi} | |\tilde{\Psi}\rangle \langle \tilde{\Psi} | \partial_\beta \tilde{\Psi} \rangle - \langle \partial_\beta \tilde{\Psi} | |\tilde{\Psi}\rangle \langle \tilde{\Psi} | \partial_\alpha \tilde{\Psi} \rangle}{\langle \tilde{\Psi} | \tilde{\Psi} \rangle^2} \right]$$

here α label the $4J$ coordinates of the $2J$ Majorana stars \mathbf{n}_i

geometrical (Berry-Aharonov-Anandan) phase for a round trip in state space:

$$\Phi_B = \oint \sum_{i=1}^{2J} \mathbf{A}_i \cdot d\mathbf{n}_i$$

\mathbf{A}_i plays the role of a vector potential for \mathbf{n}_i



$$\mathbf{A}_i = \frac{1}{4\pi} \int d\Omega P_{\tilde{\Psi}}(\Omega) \mathbf{A}_i(\Omega)$$

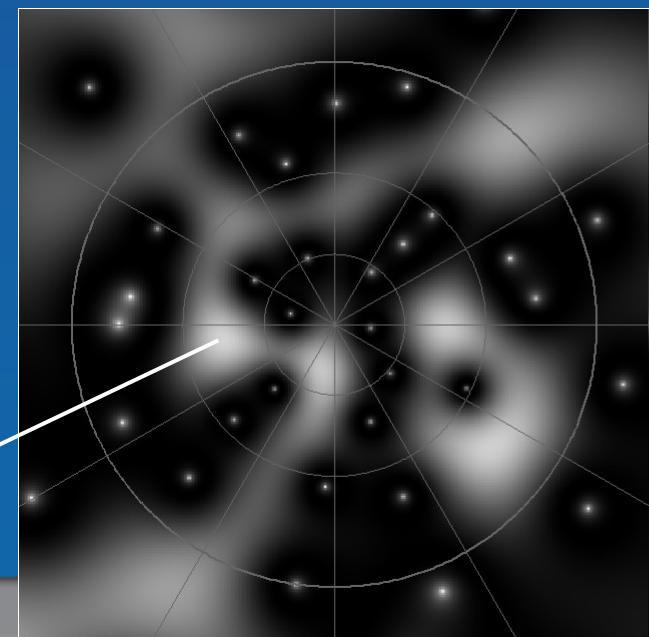
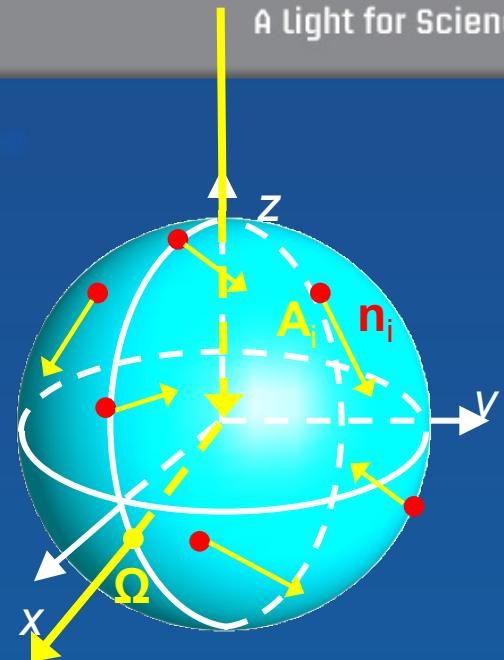
with $\mathbf{A}_i(\Omega) = \frac{1}{2} \left(\frac{\hat{\mathbf{z}} \times \mathbf{n}_i}{1 - \hat{\mathbf{z}} \cdot \mathbf{n}_i} - \frac{\Omega \times \mathbf{n}_i}{1 - \Omega \cdot \mathbf{n}_i} \right)$

= vector potential for a Dirac string carrying unit flux quantum, entering along \mathbf{z} and exiting along Ω

$$\mathbf{A}_i = \frac{1}{4\pi} \int d\Omega P_{\tilde{\Psi}}(\Omega) \mathbf{A}_i(\Omega) = \frac{1}{2} \left(\underbrace{\frac{\hat{\mathbf{z}} \times \mathbf{n}_i}{1 - \hat{\mathbf{z}} \cdot \mathbf{n}_i}}_{\text{magnetic monopole}} - \underbrace{\frac{\partial F(\tilde{\Psi})}{\partial \mathbf{n}_i} \times \mathbf{n}_i}_{\text{fictitious force acting test charge } \mathbf{n}_i} \right)$$

magnetic monopole fictitious force acting test charge \mathbf{n}_i

the flux density is given by $P_{\tilde{\Psi}}(\Omega)$



quantum dynamics

$$\sum_{j=1}^{2J} \bar{\mathbf{f}}_{ij} \cdot \frac{d\mathbf{n}_j}{dt} = \frac{\partial H(\tilde{\Psi})}{\partial \mathbf{n}_i}$$

symplectic structure
of the projective Hilbert
space

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \dot{x} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} \partial_x H \\ \partial_p H \end{pmatrix}$$

energetics
(interactions)

= generalization for a spin J of the Bloch equation of motion of a spin $\frac{1}{2}$
= quantum version of the Landau-Lifshitz (classical) equation for spin dynamics

quantum spin $J \leftrightarrow$ ensemble of $2J$ classical gyroscopes coupled through their
symplectic structure, as well as dynamically (Hamiltonian)

Towards a *Geometric Theory* of Quantum Many-Spin Systems

$\Omega_n \equiv$ unit vector of the coherent state for a spin J at site \mathbf{R}_n

partition function at temperature β^{-1} : $Z \equiv \oint \prod_n D\Omega_n(\tau) \exp(-\tilde{S}[\Omega])$

$\tau \equiv$ imaginary time

path integral over all the closed paths for the Ω_n
with the boundary condition $\Omega_n(\beta) = \Omega_n(0)$

with the action $\tilde{S}[\Omega] = -i \underbrace{\sum_n \omega[\Omega_n]}_{\text{Berry phase}} + \int_0^\beta d\tau H[\Omega(\tau)]$

$\omega[\Omega_n] \equiv$ solid angle described by Ω_n between 0 and β

describes successfully:

- spin waves in ferromagnets and antiferromagnets
- Mermin-Wagner theorem (no ordering for $T>0$, $D \leq 2$)
- Haldane gap for AF chain of integer spin
- ...

inconvenient for describing spin systems with exotic (quadupolar) ordering such as spin nematics

$\mathbf{N}_n \equiv \{\mathbf{n}_i(\mathbf{R}_n)\}$ (Majorana constellation at site \mathbf{R}_n)

partition function at temperature β^{-1} :

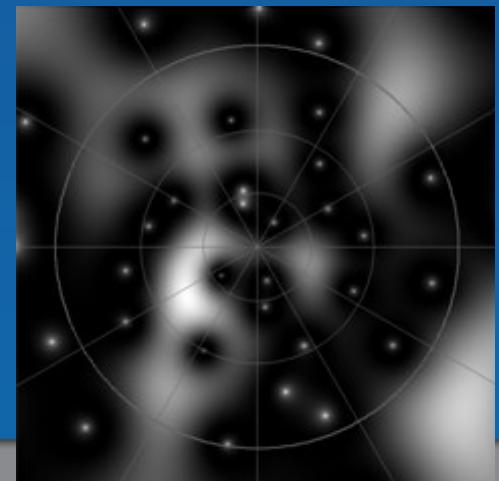
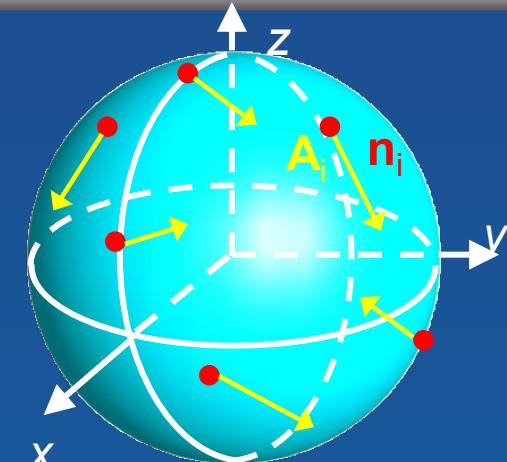
$$Z \equiv \oint \prod_n D\mathbf{N}_n(\tau) \exp(-\tilde{S}[\mathbf{N}])$$

with the boundary condition $\mathbf{N}_n(\beta) = \mathbf{N}_n(0)$

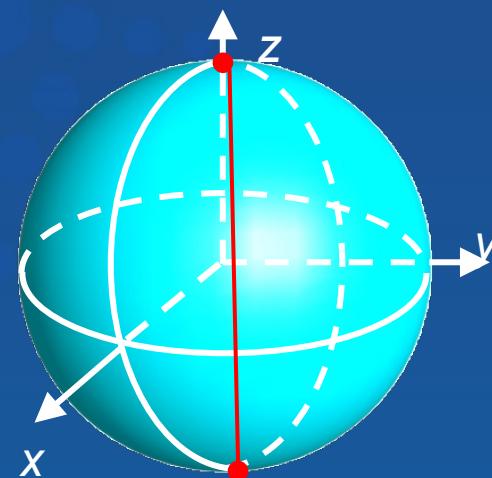
$$\text{with the action } \tilde{S}[\mathbf{N}] = \underbrace{-i \sum_n \Phi_B[\mathbf{N}_n]}_{\text{Berry phase}} - \underbrace{\frac{1}{\beta} \sum_n \int_0^\beta d\tau \ln \sqrt{\det(\bar{\mathbf{g}}(\mathbf{N}_n(\tau)))}}_{\text{quantum metric}} + \underbrace{\int_0^\beta d\tau H[\mathbf{N}(\tau)]}_{\text{dynamic action}}$$

$$\Phi_B[\mathbf{N}_n] = \oint \sum_{i=1}^{2J} \mathbf{A}_i \cdot d\mathbf{n}_i$$

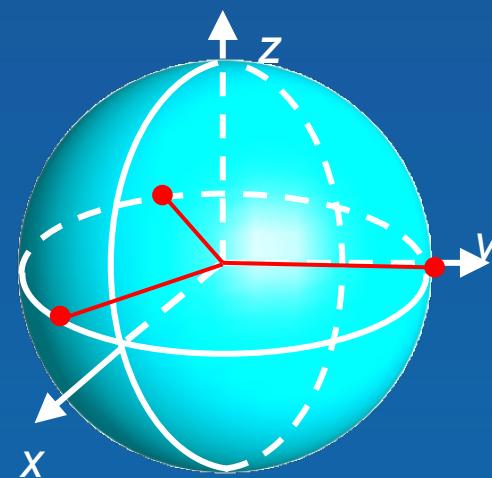
appropriate to describe spin systems with exotic ordering because the quantum state of each each spin is treated exactly



spin 1 nematic



spin 3/2 nematic



Concluding remarks and outlook

- Majorana's stellar representation allows a novel, fully geometrical, interpretation of the concept of geometrical phase for a spin system
- the geometrical representation is the most natural setting to describe the dynamics of systems such as molecular magnets
 - → quantum spin systems (chains, planes, etc...) with $J > \frac{1}{2}$ and unconventional magnetic order (quadrupole, octupole, etc...)
 - → study the interaction of X-rays and neutrons with spin systems having quadrupolar ordering (suggest methods for experimental investigation of spin nematics)

if you want to learn more about this: P.B., Phys. Rev. Lett. **108**, 240402 (2012)
see also: Physics Viewpoint "A Quantum Constellation", Physics **5**, 65 (2012)

Thank you for your attention !

