FACOLTÀ DI SCIENZE MATEMATICHE, FISICHE E NATURALI
DIPARTIMENTO DI MATEMATICA E FISICA "NICCOLÒ TARTAGLIA"
INTERNATIONAL DOCTORAL PROGRAM IN SCIENCE

GEOMETRIC METHODS IN QUANTUM MECHANICS

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Since its emergence during last century's twenties, quantum mechanics has fostered the development of both old and entirely new mathematical domains, thus providing a perennial source of fascinating research problems. The present course, mainly geared towards (but not limited to) mathematicians, is intended as a gentle introduction to the mathematical aspects of quantum mechanics, focussing on the geometrical ones. Here is a cursory and tentative list of the planned topics: quantum mechanics (overview), geometric quantum mechanics, geometric quantization and applications, geometry of the Madelung-Bohm hydrodynamical approach, abelian varieties and theta functions. Basic acquaintance with differential geometry is required; however, specific technical tools will be introduced when needed.

General references

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[2] V. Guillemin & S. Sternberg: Geometric Quantization and Multiplicities of Group Representations, Invent. math. 67 (1982), 515-538.
[3] B.C. Hall: Quantum Theory for Mathematicians, GTM 267 Springer, New York, Heidelberg, Dordrecht, London, 2013.
[4] B. Khesin, G. Misiołek & K. Modin: Geometry of the Madelung Transform, Arch. Rational Mech. Anal. 234 (2019), 549–573.
[5] F. Strocchi: An Introduction to the Mathematical Structure of Quantum Mechanics, World Scientific, Singapore, 2008.
[6] M. Spera: Geometric methods in quantum mechanics, J. Geom. Symmetry Phys. 24 (2011), 1-44, also in Proc.XIII Conference on "Geometry, Integrability and Quantization" Varna, Bulgaria, 3-8 June 2011; I. Mladenov, G. Vilasi, A. Yoshioka Eds.pp. 43-82.
[7] ------: Moment map and gauge geometric aspects of the Schroedinger and Pauli equations, Int.J.Geom.Meth.Mod.Phys. 13 (4) (2016), 1630004 (1-36).
[8] ------: On Some Geometric Aspects of Coherent States, in Coherent States and Their Applications (J-P. Antoine, F. Bagarello, J-P. Gazeau eds), Ch.8 (16 pp.) Springer Proceedings in Physics 205 (2018).
[9] ------: Some Topological Applications of Theta Functions, in Integrable Systems and Algebraic Geometry, vol. 2, Editors: R. Donagi, T. Shaska (in honour of Emma Previato) (2020), Cambridge University Press: LMS Lecture Notes Series, 440-484.

PhD Course

May 17, 18, 24, 25 2021
h. 15-17

Fai clic qui per partecipare alla riunione

UNIVERSITÀ CATTOLICA del Sacro Cuore

GEOMETRIC METHODS IN QUANTUM MECHANICS

Mauro Spera - UCSC Brescia

Lecture I

Quantum mechanics (overview)

International Doctoral Program in Science

Brescia, Capitolium

Some milestones in the development of quantum theory

- M. Planck (1900) — spectrum of blackbody radiation

  harmonic oscillator quantization

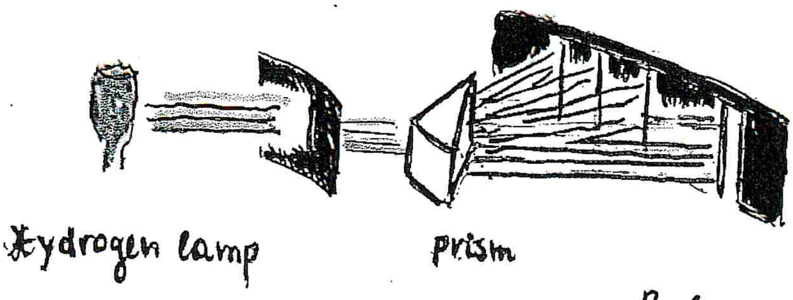
- A. Einstein (1905) — photoelectric effect

  photon $\quad E = h\nu$

- N. Bohr (1913) — quantization of energy levels in the Rutherford model of the atom (Bohr's atom)

$$E_n = -\frac{me^4}{2\hbar^2 n^2}$$

$\hbar = \frac{h}{2\pi} = 1{,}054 \cdot 10^{-27}$ erg·s



Balmer, Lyman, Paschen...

Spectroscopy — Ritz-Rydberg combination principle

$$\nu_{ij} + \nu_{jk} = \nu_{ik}$$

— A. Sommerfeld (1916) Atombau und Spektrallinien

$$\int p_i \, dq_i = n_i \hbar$$ (wrong..)

conjugate momentum position

recall

$\int_\gamma p\,dq \equiv$ action along γ

pass to

★ action - angle variables

(celestial mechanics: orbital elements)

cf. ★ stationary action principle: Euler, Maupertuis, Hamilton Jacobi

• A. Einstein (1917)

ignored for 40 years

$$\left[\underbrace{\int_{\gamma_i} \underbrace{p\,dq}_{\text{symplectic potential}}}_{I_i} = n_i \hbar \right]$$

symplectic potential

still incorrect

$+ \nu_i$

Maslov terms...

★ **Bohr - Sommerfeld quantization conditions** (OQT "old" quantum theory)

valid for **completely integrable** systems

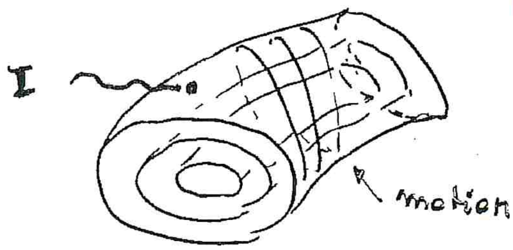
(i.e. admitting "sufficiently many" integrals of motion

almost periodic motion

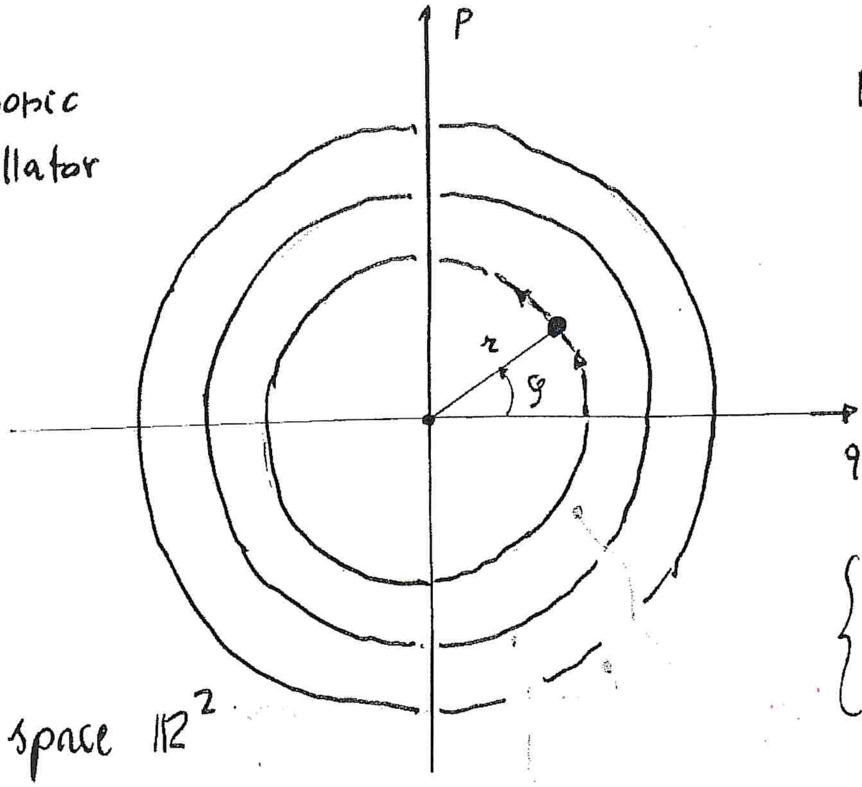
★ phase space foliated by Lagrangian tori labelled by the action variables

Liouville - Arnol'd

★ quantization : selection of suitable tori ...



Harmonic oscillator



phase space $\mathbb{R}^2$

Lagrangian torus

$H = I = r^2 =$
$= q^2 + p^2$
$\equiv$ action
$\varphi \equiv$ angle

Hamilton's equations

$$\begin{cases} \dot{I} = 0 & I = \text{const} \\ \dot{\varphi} = \frac{\partial H}{\partial I} = 1 & \text{constant speed} \end{cases}$$

BS ... radius quantization

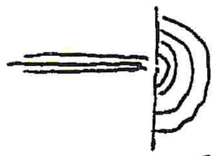
- **De Broglie** (1923) ✱ $\boxed{\text{wave-particle duality}}$

DB wavelength → $\lambda = \frac{h}{p}$ ← linear momentum

- **Compton effect**

✱ undisturbed motion: wave
✱ collision: particle

✱ diffraction of material particles



- Davisson-Germer
Thompson-Reid (1928)

W. Heisenberg
(1925)

* **matrix** mechanics

$$\dot{F} = \frac{i}{\hbar}[H, F]$$

H, **F** matrices (observables)

$$H = \begin{pmatrix} E_1 & & & 0 \\ & E_2 & & \\ & & \ddots & \\ 0 & & & E_n \end{pmatrix}$$

$$F_{mn}(t) = F_{mn}(0)\, e^{i \frac{E_m - E_n}{\hbar} t}$$

* abstract,
changes abruptly
the "rules of the game"

"QM as a non commutative phase space"

RR combination principle

Pauli

Schrödinger

$\boxed{\text{Hydrogen atom}}$

E. Schrödinger
(1926)

* **wave** mechanics

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H} \Psi$$

$\Psi = \Psi(q, t)$ wave function

$\mathcal{H}$: Hamilton operator
differential, linear

"state" of the system

superposition principle
$\Downarrow$
stationary state equation
(eigenvalue problem)

$$\mathcal{H}\Psi = E\Psi$$

$$\left(\frac{\hbar^2}{2m}\Delta - U\right)\Psi + E\Psi = 0$$

$$\Psi_n(q, t) = e^{-\frac{i}{\hbar}E_n t}\, \Psi_n(q, 0)$$

wave optics $\longleftrightarrow$ **wave mechanics**
$\downarrow \lambda \to 0$ $\quad\quad$ $\downarrow \hbar \to 0$
geometric optics $\longleftrightarrow$ classical mechanics

Hamilton

semi classical wave function

$\Psi = a\, e^{i/\hbar\, S}$

classical action

eikonal equation $\longleftrightarrow$ Schrödinger equation

* Actually, we have two facets of the same theory
(Schrödinger, von Neumann, Weyl, Dirac)

What is the meaning of ψ ?

→ A "realistic" interpretation is untenable

- **M. Born (1926)**

  ★ probabilistic interpretation of ψ

  ψ : probability amplitude

$$|\psi(q,t)|^2 \, d^3q \equiv$$

probability of finding the "particle" in

d^3q

q

at time t

$$\int_{\mathbb{R}^3} |\psi(q,t)|^2 \, d^3q = 1$$

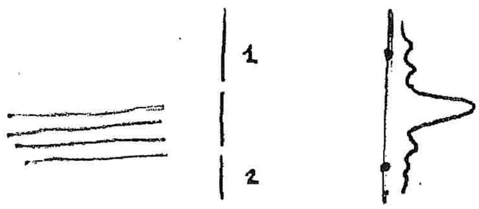
normalization

$$\psi \longmapsto e^{i\alpha}\psi \qquad \alpha \in \mathbb{R} \quad \text{(phase)}$$

leaves $|\psi|^2$ invariant

- the two-slit experiment

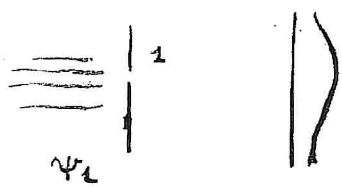
ψ_i ~ passage through slit i whilst the other is shut



$$|\psi_1+\psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + \underbrace{2\,\mathrm{Re}\,\bar{\psi}_1\psi_2}_{\text{interference}}$$

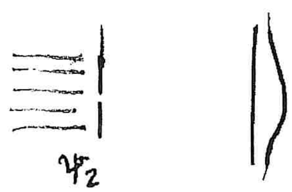
$\psi_1 + \psi_2$

superposition



ψ_1

$$|\psi_1+\psi_2|^2 \neq |\psi_1|^2 + |\psi_2|^2$$



ψ_2

★ measurement involves interaction

detection of the position determines a change of momentum
(and vice versa)

★ **Heisenberg Uncertainty Principle** (1927)

$$\Delta q \, \Delta p \approx \hbar$$

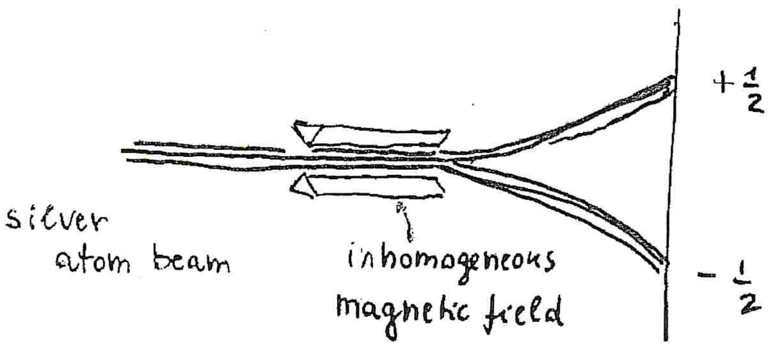
(Fourier analysis...)

(⇒ the concept of classical trajectory becomes meaningless)

- Internal degrees of freedom

  spin of the electron (W. Pauli 1927)

  intrinsic angular momentum (~ rotations)
  quantized
  no direct spatial interpretation ... no ... top model!



- O. Stern – W. Gerlach (1927)

- **Dirac** — The Principles of Quantum Mechanics (1932)

relativistic theory of the electron

★ elucidated the problem of quantization

$$\{\ ,\ \} \rightsquigarrow \frac{i}{\hbar}[\ ,\ ]$$

defined via a symplectic form

Poisson brackets — Commutator

$$\boxed{\dot{f} = \{H, f\}}$$

Hamilton equations

$$\boxed{\dot{F} = \frac{i}{\hbar}[H, F]}$$

Heisenberg equations

★ basic example — Schrödinger representation

$$\mathcal{H} = L^2(\mathbb{R}, dq)$$

$$q \rightsquigarrow Q = q\,\cdot$$

$$p \rightsquigarrow P = -i\hbar\frac{\partial}{\partial q}$$

Recall → generator of translations . . $f(x+h) = f(x) + \underbrace{f'(x)h}_{} + \ldots$

$$\boxed{[Q, P] = -i\hbar I}$$

★ canonical commutation relations

- **Born - Heisenberg - Jordan**

… replaces Bohr - Sommerfeld

Here come the mathematicians ...

- **J. von Neumann** (1932)

  Mathematische Grundlagen der Quantenmechanik

  - self-adjointness   Stone's theorem

    quantum measurement

  - **von Neumann algebras** (1936 →)

- **H. Weyl** (1931) "...the last encyclopedic mathematician. G. Fichera

  Quantenmechanik und Gruppentheorie

  gauge theory ideas

  internal degrees of freedom

  ≡ (irreducible) representations of Lie Groups

  Spin ↔ SU(2)

- Borel - Weil   geometric construction of

- Weil - Kostant

  Kirillov - Kostant - Souriau $\boxed{\text{geometric quantization}}$

  (in the Schrödinger's tradition)

exploits classical aspects

$\boxed{\text{geometric quantum mechanics}}$

quantum mechanics itself looked upon geometrically

Basic formalism of QM

- H Hilbert space $\langle \, | \, \rangle$ $H \cong H^*$
  complex, separable
  Conjugate linear — linear
  R.S.

$|v\rangle \in H$ "ket"
$\langle w| \in H^*$ "bra"

$\langle w | v \rangle$
bra - ket
(c)

$S(H)/\sim \;\equiv$ pure **states** of the system $([v])$

$\|v\| = 1$ $\quad v \sim e^{i\alpha} v$

$(\equiv \mathbb{P}(H))$
projective space

Self-adjoint operators on H $\equiv$ **observables**

in principle, due to the spectral theorem it is enough to restrict to bounded operators (everywhere defined)

$A = A^*$

$\bar{A} := \langle v | A v \rangle \quad (\in \mathbb{R})$

mean value of A in the state $[v]$

★ variance (dispersion)
uncertainty of A in $[v]$

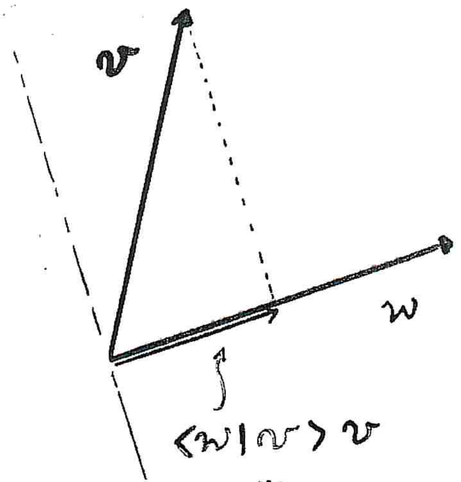
$$\Delta_{[v]}(A) = \| Av - \langle v | A v \rangle v \|$$
$$\equiv \left(\bar{A^2} - \bar{A}^2 \right)^{1/2}$$

$\langle w | v \rangle$

transition amplitude
(from $[v]$ to $[w]$)
defined up to phase

$|\langle w | v \rangle|^2$

transition probability
from $[v]$ to $[w]$
i.e. probability of finding $[v]$ in $[w]$
(intrinsic)



$\langle w | v \rangle v$

$\equiv$

$|v\rangle \underbrace{\langle w | v \rangle}_{\text{transition amplitude}}$

$|\langle w | v \rangle|^2 \equiv$ length (squared) of orthogonal projection of v onto $\langle w \rangle$

orthogonality $\equiv$ no correlation

★ unitary dynamics : $\mathcal{H}$ Hamiltonian

$$|v\rangle \longmapsto U(t)|v\rangle = e^{-\frac{i}{\hbar}\mathcal{H}t}|v\rangle$$

(Schrödinger) (Stone's theorem) one-parameter unitary group

$$\mathcal{H} = \sum E_i \underbrace{|e_i\rangle\langle e_i|}_{P_i}$$

$\mathcal{H} e_i = E_i e_i$

orthonormal basis of eigenvectors

★ spectral theorem (von Neumann)

confining ourselves to point spectrum operators...

projection onto $\langle e_i \rangle$

$$\mathcal{H} = \begin{pmatrix} E_1 & & 0 \\ & E_2 & \\ 0 & & \ddots \end{pmatrix}$$

$[e_i]$: stationary states

E_i : measured values

if $v = \sum \alpha_i e_i$ $\quad \sum|\alpha_i|^2 = 1$

superposition

$$\langle v | H v\rangle = \sum E_i |\alpha_i|^2$$

★ upon measuring an observable in $[v]$, say $\mathcal{H}$ one finds E_i with probability $|\alpha_i|^2$

(requires an ensemble) $\quad |\alpha_i|^2 = |\langle e_i | v\rangle|^2$

$$|v\rangle\langle v| = \dots = \sum \bar{\alpha}_i \alpha_j \, |e_i\rangle\langle e_j|$$

$$(\bar{\alpha}_i \alpha_j) = \begin{pmatrix} |\alpha_1|^2 & & \bar{\alpha}_i\alpha_j \\ & |\alpha_2|^2 & \\ & & \ddots \end{pmatrix}$$

interference terms

density matrices

$$\rho := \sum_i |\alpha_i|^2 \, |e_i\rangle\langle e_i|$$

$$\rho = \begin{pmatrix} |\alpha_1|^2 & & 0 \\ & |\alpha_2|^2 & \\ 0 & & \ddots \end{pmatrix}$$

⚠ quite different!

→ describes a <u>mixed state</u>
(assembly of states in proportions $|\alpha_i|^2$)

$$|v\rangle\langle v| \xrightarrow{\text{measurement}} \rho \quad \text{mixed}$$

superposition (pure state) — interference destroyed

★ moreover: "collapse of the wave function"
looking upon a single process

$$v = \sum \alpha_i e_i \rightsquigarrow \underline{e_j}$$

(**incompatible** with a Schrödinger evolution of the system + apparatus)
$\qquad S + A$

[**decoherence** : consider $S + A + E$]
$\qquad E$: environment

Zeh, Zurek, Joos.... ⇒ explain the classical appearance of reality

★ Heisenberg uncertainty principle ($\hbar = 1$)
(becomes a theorem)

$$\Delta_{[v]}(A) \cdot \Delta_{[v]}(B) \geq \frac{1}{2} |\langle v | [A,B] v \rangle|$$

A and **B** simultaneously measurable iff they **commute** ($[A,B] = 0$) $\Leftrightarrow$
they are simultaneously diagonalizable
(i.e. with respect to the **same** orthonormal basis)

◆ Symmetries

Lie group, unitary operators

$$\rho : G \longrightarrow U(H)$$

$$\rho(g \cdot g') = \rho(g)\,\rho(g')$$

decompose into

$$\rho(1) = \mathbb{1}$$

ρ : irreducible unitary representation

no subspace left invariant...

$$\Rightarrow \quad |\langle \rho(g) w \mid \rho(g) v \rangle|^2 = |\langle w \mid v \rangle|^2$$

E. Noether (1916)

symmetries
$\updownarrow$
conservation laws

- linear momentum
- translations

- angular momentum
- rotations

in the Lagrangian setting

Hamiltonian setting **moment map**

conversely, any transformation preserving transition probabilities is induced by a unitary (or antiunitary) operator (**Wigner's theorem**)

** Heisenberg - Weyl

Q_j: position
P_k: momentum

$$\boxed{\begin{aligned}[Q_i, Q_j] &= [P_i, P_j] = 0 \\ [Q_j, P_k] &= i\,\delta_{jk} I\end{aligned}}$$

$U(\alpha) = e^{i \sum \alpha_j Q_j}$

$V(\beta) = e^{i \sum \beta_j P_j}$

$\alpha = (\alpha_1 \dots \alpha_n)$
$\beta = (\beta_1 \dots \beta_n)$

annihilation & creation operators

$$A_j = \frac{1}{\sqrt{2}} (Q_j + i P_j)$$

$$A_j^{\dagger} = \frac{1}{\sqrt{2}} (Q_j - i P_j)$$

$$\boxed{\begin{aligned}[A_j, A_k] &= [A_j^{\dagger}, A_k^{\dagger}] = 0 \\ [A_j, A_k^{\dagger}] &= \delta_{jk} I\end{aligned}}$$

$$(*) \quad \boxed{V(\beta) U(\alpha) = e^{i \alpha \cdot \beta} U(\alpha) V(\beta)}$$

Weyl form on a Hilbert space $\mathcal{H}$

* von Neumann uniqueness theorem

up to unitary equivalence, there is only one irreducible representation of $(*)$, characterized by the fact that $\bigcap_{j=1}^{n} \operatorname{Ker} A_j$ is one-dimensional

e.g. Schrödinger representation

a Gaussian in the Schrödinger representation

ground state space of the quantum harmonic oscillator

with Hamiltonian

zero point energy

$$\boxed{H = \frac{1}{2} \sum P_j^2 + Q_j^2 = \sum A_j^{\dagger} A_j + \frac{n}{2} I}$$

Eigenvectors:

$$\prod_{j=1}^{n} (k_j!)^{-\frac{1}{2}} (A_j^+)^{k_j} \Phi_0$$

$A^+ \Gamma^\cdot \Phi_0$

eigenvalues: $\sum_{j=1}^{n} (k_j + \frac{1}{2})$

$\rightsquigarrow$ QFT

$$\Phi_{\alpha\beta} := U(\alpha,\beta)\,\Phi_0 \equiv e^{i\,\Sigma(\alpha_j Q_j - \beta_j P_j)}\,\Phi_0$$

* Coherent states

$\Phi_{\alpha\beta}$: ground state of the displaced quantum oscillator Hamiltonian

$$H_{\alpha\beta} = \frac{1}{2}\sum_j (Q_j - \alpha_j I)^2 + (P - \beta_j I)^2$$

$\Phi_{\alpha\beta}$ yield the eigenvectors of A_j

$$A_j \Phi_{\alpha,\beta} = \frac{1}{\sqrt{2}}(\alpha_j + i\beta_j)\,\Phi_{\alpha\beta}$$

Also minimal uncertainty wave packets et cetera...

The Bargmann - Fock representation

$$\mathcal{H} = \left\{ f \text{ holomorphic} \;\middle|\; \int_{\mathbb{C}} e^{-|z|^2} |f(z)|^2 \, dx\,dy < \infty \right\}$$

it is already a Hilbert space

$$a = \frac{\partial}{\partial z} \qquad a^+ = z \cdot$$

$$(*) \qquad [a, a^+] = I$$

$|0\rangle \equiv 1$: ground state of the QHO

orthonormal basis (up to constants)

$$(a^+)^n |0\rangle \longleftrightarrow z^n$$

$$' = \frac{d}{dz}$$

$$(*) \quad (aa^+ - a^+a)\psi = (z\psi)' - z\psi' = z'\psi + z\psi' - z\psi'$$
$$= \psi$$

Schrödinger

real polarizations

$\Downarrow$

Bohr-Sommerfeld quantization

Bargmann-Fock

Complex polarization

$\Downarrow$

holomorphic (Kähler) quantization

Spin (standard treatment)

$$SU(2) \xrightarrow{2:1} SO(3) \qquad \dim \overset{\text{spin space}}{\bar{V}_j} = 2j+1 \qquad j \in \frac{\mathbb{Z}}{2}$$

raising (+) & lowering (−) operators

$$J_\pm = J_1 \pm i J_2$$

1, 2, 3 : space directions

$$J_0 = J_3$$

$|j,\mu\rangle \quad \mu = -j, \dots j$

orth. basis : eigenvectors of J_0

$$J_+ | j,\mu\rangle = \sqrt{(j-\mu)(j+\mu+1)}\ |j,\mu+1\rangle$$

$$J_- | j,\mu\rangle = \sqrt{(j+\mu)(j-\mu+1)}\ |j,\mu-1\rangle$$

$$J_- | j,-j\rangle = 0 \qquad J_0 |j,\mu\rangle = \mu |j,\mu\rangle$$

"lowest weight vector"

$$[J_0, J_\pm] = \pm J_\pm$$

$$[J_-, J_+] = -2J_0$$

$$|j,\mu\rangle = \sqrt{\frac{(j-\mu)!}{(j+\mu)!\,(2j)!}}\ J_+^{\,j+\mu}\ |j,-j\rangle$$

$\rightsquigarrow$

Borel–Weil