Bohr-Sommerfeld Quantum Systems

Shifting Operators

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Bohr-Sommerfeld theory of a completely integrable system

- Phase space $P = T^*\mathbb{R}^k$ with coordinates $(p_i, q_i) \equiv (\mathbf{p}, \mathbf{q})$,

$$\omega = \sum_i dp_i \wedge dq_i = d\mathbf{p} \wedge d\mathbf{q}.$$

- $(f_1, ..., f_k)$ inedpendent functions on P.
- $D = \mathrm{span}\left(X_{f_1}, ..., X_{f_k}\right)$.

Theorem

Quantum states of the system are concentated on integral manifolds M of D such that, for every closed loop $\gamma : S^1 \to M \subset T^*\mathbb{R}^3$, there exists an integer n such that

$$\oint \gamma^* \mathbf{p} d\mathbf{q} = nh,$$

where h is Planck's constant.

- Compact Integral manifolds M of D satisfying Bohr-Sommerfeld conditions are called Bohr-Sommerfeld.
- We denote by $\mathfrak{B}$ the set of of Bohr-Sommerfeld tori.

Fate of Bohr-Sommerfeld theory

- In 1915, A. Sommerfeld applied it to the bounded states of the relativistic hydrogen atom. His result are in exact agreement with observations.
- Attempts to apply Bohr-Sommerfeld theory to helium atom failed to provide useful results.
- In 1925, Heisenberg criticized Bohr-Sommerfeld theory for not providing transition operators between different states.
- For a long time the Bohr-Sommerfeld theory has been known mainly for its agreement with the quasi-classical limit of Schrödinger theory.
- Nevertheless, it has been consistently used by quantum chemists in their study of chemical bonds..
- In 1975, I showed that Bohr-Sommerfeld conditions are necessary and sufficient conditions for existence of sections of the prequantization line bundle that are covariantly constant along integral manifolds M of D.

Geometric quantization in a toric polarization.

- Assume that integral manifolds of $D = \mathrm{span}\,(X_{f_1}, ..., X_{f_k})$ are Lagrangian k-tori in (P, ω).
- $\pi : L \longrightarrow P$ is the prequantization line bundle of (P, ω).
- $\pi^{\times} : L^{\times} \longrightarrow P$ is the associated principal fibre bundle of L; it may be visualized as L with zero section removed.
- For each $f \in C^{\infty}(P)$ there exists a vector field Z_f on $L^{\times}$, $\pi^{\times}$-related to X_f, preserving the connection form.
- The flow of Z_f on $L^{\times}$ is the parallel transport along integral curves of X_f multiplied by a phase factor.

$$\mathrm{e}^{tZ_f} = \mathrm{e}^{-2\pi i t f/h} \mathrm{e}^{t \mathrm{lift} X_f} \tag{1}$$

- The space $\mathfrak{S}$ of sections σ of L that are covariantly constant along D, is supported on the union of Bohr-Sommerfeld tori.
- For $i = 1, ..., n$, the quantum operator $\mathbf{Q}_f$ acting on $\sigma \in \mathfrak{S}$ is

$$\mathbf{Q}_f \sigma = i\hbar \frac{d}{dt} \left(\mathrm{e}^{tZ_f} \right)_* \sigma = f\sigma. \tag{2}$$

Action angle coordinates

- Action angle coordinates $(\mathbf{j}, \boldsymbol{\vartheta}) = (j_1, .., j_k, \vartheta_1, .., \vartheta_k)$ are maps from an open set U in P to $\mathbb{R}^k \times \mathbb{T}^k$, where each $\vartheta_i : U \to \mathbb{T} = \mathbb{R}/\mathbb{Z}$ is interpreted as a multi-valued real function, such that

$$\omega_{|U} = \sum_{i=1}^{k} \mathrm{d}j_i \wedge \mathrm{d}\vartheta_i. \tag{3}$$

- In action-angle coordinates $(j_1, .., j_k, \vartheta_1, .., \vartheta_k)$, Bohr-Sommerfeld tori are given by equations

$$j_i = n_i h, \tag{4}$$

  where n_i are integers.
- If the domain U' of $(\mathbf{j}', \boldsymbol{\vartheta}') = (j'_1, .., j'_k, \vartheta'_1, .., \vartheta'_k)$ has non empty intersection with U then, in $U \cap U'$,

$$j_i = \sum_{l=1}^{k} a_{il} j'_l \quad \text{and} \quad \vartheta_i = \sum_{l=1}^{k} a_{il} \vartheta'_l. \tag{5}$$

  where $A = (a_{ij})$ and $B = (b_{ij})$ have integer entries, and $B = (A^{-1})^T$.

Shifting operators

The simplest case

- $U = \mathbb{R}^k \times \mathbb{T}^k$, $\omega = \sum_{i=1}^k \mathrm{d}j_i \wedge \mathrm{d}\vartheta_i$. For each $i = 1, ..., k$ set $X_i = -\frac{\partial}{\partial j_i}$.

$$X_i \lrcorner \omega = -d\vartheta_i$$

is well defined. Since ϑ_i is multi-valued, X_i is a local Hamiltonian vector field and ϑ_i gives it local Hamiltonians.

- Equation (1) with $f = \vartheta_i$ is multi-valued because the phase factor is multivalued,

$$\mathrm{e}^{tZ_{\vartheta_i}} = \mathrm{e}^{-2\pi i t\vartheta_i/h} \mathrm{e}^{t\mathrm{lift}X_i}. \tag{6}$$

- If $t = h$, then

$$\mathrm{e}^{hZ_{X_i}} = \mathrm{e}^{-2\pi i\vartheta_i} \mathrm{e}^{h\mathrm{lift}X_i} \tag{7}$$

is well defined. It depends only on X_i and not the choice of the local Hamiltonian ϑ_i.

- One could use covering of $\mathbb{T}^k$ by contractible open sets V_α, take $W_\alpha = U\times\ V_\alpha$ and in each W_α choose a representative $\theta_{i\alpha}$ of $\vartheta_{i|W_\alpha}$ to obtain the same result.

- Note that

$$\mathrm{e}^{hZ_{X_i}} : L^{\times} \to L^{\times} : l^{\times} \mapsto \mathrm{e}^{hZ_{X_i}} l^{\times} = \mathrm{e}^{-2\pi i \vartheta_i} \mathrm{e}^{h \mathrm{lift} X_i} l^{\times} \tag{8}$$

- is the unique lift of the symplectomorphism $\mathrm{e}^{hX_i} : U \to U$ to a connection preserving automorphism of the prequantization line bundle
- Since $L = (L^{\times} \times \mathbb{C})/\mathbb{C}^{\times}$, the action of $\mathrm{e}^{hZ_{X_i}}$ on $L^{\times}$ gives an action

$$\mathrm{e}^{hZ_{X_i}} : L \to L : l = [l^{\times}, c] \mapsto [(\mathrm{e}^{hZ_{X_i}} l^{\times}, c)]. \tag{9}$$

- The automorphism $\mathrm{e}^{hZ_{X_i}}$ of L acts on sections of $\pi : L \to U$ by pull-backs and push-forwards

$$\begin{aligned} \left(\mathrm{e}^{hZ_{X_i}}\right)_* \sigma(p) &= \mathrm{e}^{-hZ_{X_i}} \left(\sigma\left(\mathrm{e}^{hX_i}(p)\right)\right) \\ &= \mathrm{e}^{-2\pi i \vartheta_i} \cdot \mathrm{e}^{-h\mathrm{lift} X_i} \left(\sigma\left(\mathrm{e}^{hX_i}(p)\right)\right), \\ \left(\mathrm{e}^{hZ_{X_i}}\right)^* \sigma(p) &= \mathrm{e}^{hZ_{X_i}} \left(\sigma\left(\mathrm{e}^{-hX_i}(p)\right)\right) = \\ & \mathrm{e}^{2\pi i \vartheta_i} \cdot \mathrm{e}^{h\mathrm{lift} X_i} \left(\sigma\left(\mathrm{e}^{-hX_i}(p)\right)\right) \end{aligned} \tag{10}$$

Theorem

The linear maps $\sigma \mapsto \left(\mathfrak{e}^{hZ_{X_i}}\right)_* \sigma$ and $\sigma \mapsto \left(\mathfrak{e}^{hZ_{X_i}}\right)^* \sigma$ preserve the space $\mathfrak{S}$ of Bohr-Sommerfeld quantum states. Their restrictions to $\mathfrak{S}$ generate a representation on $\mathfrak{S}$ of the group of symmetries of the lattice of Bohr-Sommerfeld tori.

- If $\sigma \in \mathfrak{S}$ is an eigenvector of $\mathbf{Q}_{j_i}$ with egenvalue $n_i h$, then,

$$\begin{aligned} \mathbf{Q}_{j_i} \left(\mathfrak{e}^{hZ_{X_i}}\right)_* \sigma &= (n_i - 1)h \left(\mathfrak{e}^{hZ_{X_i}}\right)_* \sigma \\ \mathbf{Q}_{j_i} \left(\mathfrak{e}^{hZ_{X_i}}\right)^* \sigma &= (n_i + 1)h \left(\mathfrak{e}^{hZ_{X_i}}\right)^* \sigma. \end{aligned} \tag{11}$$

- $$\left(\mathfrak{e}^{hZ_{X_i}}\right)^* = \left[\left(\mathfrak{e}^{hZ_{X_i}}\right)_*\right]^{-1} = \left(\mathfrak{e}^{hZ_{-X_i}}\right)_* . \tag{12}$$

- For $i, j = 1, ..., k$, the operators $\left(\mathfrak{e}^{hZ_{X_i}}\right)_*$, $\left(\mathfrak{e}^{hZ_{X_j}}\right)_*$, $\left(\mathfrak{e}^{hZ_{X_i}}\right)^*$ and $\left(\mathfrak{e}^{hZ_{X_j}}\right)^*$ commute with each other.

- We refer to operators $\left(\mathrm{e}^{hZ_{X_i}}\right)_*$ and $\left(\mathrm{e}^{hZ_{X_i}}\right)^*$, $i = 1, ..., k$, as shifting operators.
- Given non-zero $\sigma \in \mathfrak{S}$, supported on a Bohr-Sommerfeld torus M, the family of sections

$$\left\{ \left(\mathrm{e}^{hZ_{X_k}}\right)_*^{n_k} .... \left(\mathrm{e}^{hZ_{X_1}}\right)_*^{n_1} \sigma \in \mathfrak{S} \mid n_1, ..., n_k \in \mathbb{Z} \right\} \tag{13}$$

  is a linear basis of $\mathfrak{S}$ invariant under the action of shifting operators.
- There exists a positive definte, Hermitian scalar product $\langle \cdot \mid \cdot \rangle$ on $\mathfrak{S}$, invariant under the action of shifting operators. It is defined up to a constant positive real factor.
- With this scalar product, the basis above is orthonormal.
- The completion of $\mathfrak{S}$ with respect to this scalar product is the Hilbert space $\mathfrak{H}$ of quantum states of geometric quantization of $\left(\mathbb{R}^k \times \mathbb{T}^k, \ \sum_{i=1}^k \mathrm{d}j_i \wedge \mathrm{d}\vartheta_i\right)$ in the toral polarization given by the projection $\mathbb{R}^k \times \mathbb{T}^k \to \mathbb{R}^k$.

General case

- Writing equation $X \lrcorner \omega = -\mathrm{d}\vartheta_i$ in action-angle coordinates $(j_1', ..., j_k', \vartheta_1', ..., \vartheta_k')$, we get

$$X \lrcorner \omega = -\mathrm{d}\left(\sum_{l=1}^{k} a_{il}\vartheta_l'\right),$$

  where $a_{i1}, ..., a_{ik}$ are integers.

- On a general symplectic manifold (P, ω) with toric polarization, we consider locally Hamiltonian vector fields X such that for any action-angle coordinates $(j_1, ..., j_k, \vartheta_1, ..., \vartheta_k)$ with domain $U \subseteq P$,

$$X_{|U} \lrcorner \omega = -\mathrm{d}\varphi, \text{ where } \varphi = \sum_{i=1}^{k} a_1\vartheta_1 \text{ and } a_i \in \mathbb{Z}. \tag{14}$$

- We assume that the locally Hamiltonian vector field X in equation (14) is complete.

- Starting with $p \in U$, we follow the integral curve $\mathrm{e}^{tX}(p)$ and consider, for $I^\times \in (\pi^\times)^{-1}(p)$,

$$\mathrm{e}^{tZ_\varphi}(I^\times) = \mathrm{e}^{-2\pi i t\varphi/h}\mathrm{e}^{t\mathrm{lift}X}(I^\times). \tag{15}$$

- If $\mathrm{e}^{tX}(p) \in U$ for $t \in [0, h]$, then $\mathrm{e}^{hZ_X}(I^\times) = \mathrm{e}^{-2\pi i\varphi}\mathrm{e}^{h\mathrm{lift}X}(I^\times)$ is well defined, because φ is defined up to integer.
- If $\mathrm{e}^{hX}(p) \notin U$, but $\mathrm{e}^{hX}(p)$ is in the domain U' of action-angle coordinates $(j_1', ..., j_k', \vartheta_1', ..., \vartheta_k')$ such that $\mathrm{e}^{tX}(p) \in U \cup U'$ for $t \in [0, h]$, then follow the steps below.
- Choose a point $t_1 \in [0, h]$ such that $\mathrm{e}^{tX}(p) \in U$ for $t \in [0, t_1]$, and $\mathrm{e}^{tX}(p_1) \in U'$ for $t \in [0, h - t_1]$, where $p_1 = \mathrm{e}^{t_1 X}(p)$.
- Choose $\varphi' = a_1'\vartheta_1' + ... + a_k'\vartheta_k'$ such that $X_{|U'} \lrcorner \omega = -\mathrm{d}\varphi'$. Make sure that $\varphi'(p_1) = \varphi(p_1)$.

- Then,

$$\begin{aligned} & \mathrm{e}^{hZ_X}\left(I^\times\right) = \mathrm{e}^{(h-t_1)Z_{\varphi'}}\left(\mathrm{e}^{t_1 Z_\varphi}(I^\times)\right) = \\ = \; & \mathrm{e}^{-2\pi i(h-t_1)\varphi'/h}\mathrm{e}^{(h-t)_1 \mathrm{lift}X}(\mathrm{e}^{-2\pi i t_1\varphi/h}\mathrm{e}^{t_1 \mathrm{lift}X}(I^\times)) = \\ = \; & \mathrm{e}^{-2\pi i(h-t_1)\varphi'(p_1)/h}\mathrm{e}^{-2\pi i t_1\varphi(p_1)/h}\mathrm{e}^{(h-t)_1 \mathrm{lift}X}(\mathrm{e}^{t_1 \mathrm{lift}X}(I^\times)) = \\ = \; & \mathrm{e}^{-2\pi i\varphi'(p_1)}\mathrm{e}^{-2\pi i t_1(\varphi(p_1)-\varphi'(p_1))/h}\mathrm{e}^{h \mathrm{lift}X}(I^\times) = \\ = \; & \mathrm{e}^{-2\pi i\varphi'(p_1)}\mathrm{e}^{h \mathrm{lift}X}(I^\times) \end{aligned}$$

  is well defined and it does not depend on the intermediate point $p_1 = \mathrm{e}^{t_1 X}(p)$.
- If several intermediate action-angle coordinate charts are needed, repeat the argument above as required.
- If the vector field X is complete, we obtain globally defined shifting operators $\left(\mathrm{e}^{hZ_X}\right)_*$ and $\left(\mathrm{e}^{hZ_X}\right)^*$.
- If we have k independent, complete, locally Hamiltonian vector fields on (P, ω), which satisfy equation (14), and the lattice $\mathfrak{B}$ is connected, then there exists a Hernitian scalar product $\langle \cdot \mid \cdot \rangle$ invariant under the action of shifting operators $\left(\mathrm{e}^{hZ_{X_i}}\right)_*$ and $\left(\mathrm{e}^{hZ_X}\right)^*$.

When things go wrong

- **Monodromy**.
  - In presence of monodromy, there may exist a loop in the lattice of Bohr-Sommerfeld tori, such that for some $M \in \mathfrak{B}$,
$$\left(\mathrm{e}^{hX_{\alpha_N}} \circ .... \circ \mathrm{e}^{hX_{\alpha_1}}\right)_{|M} : M \to M$$
need not be the identity on M.
  - In this case, there is a phase factor $\mathrm{e}^{i\alpha}$ such that
$$\left(\mathrm{e}^{hZ_{X_{\alpha_N}}} \circ .... \circ \mathrm{e}^{hZ_{X_{\alpha_1}}}\right)_* \sigma_M = \mathrm{e}^{i\alpha}\sigma_M.$$
- **Incompleteness of** X.
  - If the locally Hamiltonian vector field X satisfying equation (14) incomplete, then e^{hX} is not globally defined. If the integral curve $\mathrm{e}^{tX}(p)$ is defined only for $t \in (t_{\min}, t_{\max})$, then $\mathrm{e}^{hX}(\mathrm{e}^{tX}(p))$ is defined for $t \in (t_{\min}, t_{\max} - h)$, and $\mathrm{e}^{-hX}(\mathrm{e}^{tX}(p))$ is defined for $t \in (t_{\min} + h, t_{\max})$.

THANK YOU FOR YOUR ATTENTION