Separability and Quantum Mechanics

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Summary

1. Separability: some basic concepts.
2. Separable & non-separable Hilbert spaces.
3. Separability, QFT and QM.
   - Non-equivalent representations of the CCR's in QM.
4. Polymer Quantum Mechanics.
5. The polymerized harmonic oscillator re-revisited.
   - Energy spectrum: bands.
   - Statistical mechanics.
6. Comments (relevance for LQG and LQC).

Purpose of the talk

- Discuss the physical role of separability in QFT & QM.
- Consequences of trying to use non-separable *Physical* Hilbert spaces.

Separability: a topological concept

$(X, \mathcal{T})$ topological space is **separable** if it has a **dense**, **countable** subset.

Useful characterizations:

- It is possible to find a **countable** subset $Y \subset X$ such that $\overline{Y} = X$.
- **Second countable** spaces (i.e. those with countable basis) are **always separable** [take a basis V_n, $n \in \mathbb{N}$, choose $x_n \in V_n$ for each $n \in \mathbb{N}$ and consider $Y = \cup_{n\in\mathbb{N}}\{x_n\}$ which is obviously countable and dense].
- In metrizable spaces **separability** is equivalent to **second countability**.

Examples:

- Any **finite** topological space.
- $(\mathbb{R}, \mathcal{T}_u)$, i.e. the **reals with the standard topology** $[\overline{\mathbb{Q}} = \mathbb{R}]$.
- $(X, \mathcal{T}_{\mathrm{trivial}})$ is separable (for *any* X); $[\overline{Y} = X\ \forall Y \subset X,\ Y \neq \emptyset]$.
- $C([0,1])$ with the metric topology defined by the distance $d(f,g) = \sup_{x\in[0,1]}|f(x) - f(y)|$, $[\overline{\mathbb{Q}[x]} = C([0,1])]$.
- $(X, \mathcal{T}_{\mathrm{discrete}})$ with X **uncountable** is **non-separable** (every proper subset of X is closed).

Separability & Hilbert spaces

Hilbert spaces are particular examples of topological spaces with open sets buit as union of balls $B_r(x_0) = \{x \in \mathcal{H} : \|x - x_0\| < r\}$.

A useful characterization of separable Hilbert spaces: A **Hilbert space** $\mathcal{H}$ is **separable** iff it has a **countable complete orthonormal set**. Remember $\{v_j\}$ with $j \in J$ is and orthonormal basis if:

- $\langle v_i, v_j \rangle = \delta_{ij}, \forall i, j \in J$.
- $\overline{\mathrm{span}\{v_j\}_{j\in J}} = \mathcal{H} \Leftrightarrow \mathrm{span}\{v_j\}_{j\in J}$ dense in $\mathcal{H}$.

Comments

- All **infinite dimensional**, **separable**, complex Hilbert spaces are isometrically isomorphic to $\ell^2(\mathbb{N}) := \{(a_n)_{n\in\mathbb{N}} : a_n \in \mathbb{C}, \sum_{n\in\mathbb{N}} |a_n|^2 < \infty\}$.
- Countable direct sums of separable Hilbert spaces are separable.
- In particular, Fock spaces built from separable one-particle Hilbert spaces are separable.

Separability and QFT

- One could naively expect to need "bigger" Hilbert spaces in QFT but traditional axiomatic approaches to QFT (Wightman) rely on **separable** Hilbert spaces.
- In fact, after some discussion Streater and Wightman state that:

  "All these arguments make it clear that there is no evidence that separable Hilbert spaces are not the natural state spaces for quantum field theory." [Streater and Wightman in *PCT, Spin and Statistics, and All That*, Princeton University Press (2000).]

  (Obviously they did not have LQG in mind...)

- Tensor products of **countably many separable Hilbert spaces** of dimension higher than one are not separable (mentioned also by Streater and Wightman, see also Wald's book on QFT in curved spacetimes).
- These could be natural choices to quantize an infinite chain of qbits.

Separability and QFT (continued)

- Observables involving all the particles can only be defined on separable subspaces of the full tensor product.

  "Thus, while it may be a matter of convenience to regard this state space as part of an infinite tensor product, it is not necessary." (Streater and Wightman, *ibid.*)

- The most well-known and widespread application of non-separable Hilbert spaces is certainly within LQG & LQC.

What about Quantum Mechanics?

Separability & QM

- **Separability** appears **explicitly** in the postulates of quantum mechanics. von Neumann mentions it in his formalization of the mathematical basis of QM (his *Mathematical Foundations of Quantum Mechanics*).
- There are not many reasons to renounce this (simplifying) assumption, but, from a foundational/phylosophical/interpretational point of view it is interesting to see what happens if we drop it.
- Mathematicians have studied the Schrödinger eq. in non-separable Hilbert spaces since the sixties (Burnat, Krupa, Zawisza, Chojnacki,...).
- Halvorson (a Philosopher/Mathematician) [circa 2001] discussed the Bohr complementarity principle fron this perspective.
- **Bohr complementarity principle:** A particle can never have **both** a sharp position and a **sharp** momentum.
- This principle can be contemplated from the perspective of the existence of representations of the CCR's.
- It is possible to introduce a framework where particles can **either** have precise positions **or** precise momenta.

Key idea

Circumvent the conclusions of the Stone-von Neumann theorem (regarding the uniqueness of the Schrödinger representation of the CCR's) by relaxing a **crucial hypothesis**: the **separability** of the representation Hilbert space.

Once this is done it is possible to build concrete representations of the CCR's capable of allowing states with **precise** position **or** momentum values .

Comments

- A detailed discussion of measurement issues is necessary because finite experimental resolution implies that it is impossible to measure "absolutely sharp" positions (notice, however, that we have no such qualms regarding precise energy measurements, say in atomic systems).
- The loss of uniqueness in the representations of the CCR's is familiar from standard QFT.

- A useful **non-separable** complex Hilbert space where non-unitary representations of the CCR's in Weyl form can be easily built is

$$\ell^2(\mathbb{R}) := \{\Psi : \mathbb{R} \to \mathbb{C} : \sum_{x\in\mathbb{R}} |\Psi(x)|^2 < \infty\}$$

with scalar product $\langle \Psi_1, \Psi_2 \rangle_{\ell^2(\mathbb{R})} = \sum_{x\in\mathbb{R}} \overline{\Psi_1(x)}\Psi_2(x)$.

- As the sums extend over **the whole real line**, the set $\{x \in \mathbb{R} : \Psi(x) \neq 0\}$ must be **finite** or **countable** for each $\Psi \in \ell^2(\mathbb{R})$.

Theorem (Halvorson, 2001)

The **Weyl algebra**, $U(p)V(q) = e^{-ipq}V(q)U(p)\,, \forall q, p \in \mathbb{R}$, admits **unitarily inequivalent** irreducible representations in $\ell^2(\mathbb{R})$.

Representations of the Weyl algebra

Position representation on $\ell^2(\mathbb{R})$

$$\boldsymbol{U}(p)\delta_{q_0} := e^{ipq_0}\delta_{q_0}\,, \quad \boldsymbol{V}(q)\delta_{q_0} := \delta_{q_0-q}\,, \quad \forall p, q, q_0 \in \mathbb{R}$$

- $q \mapsto \boldsymbol{V}(q)$ is not weakly continuous (no momentum operator).
- $p \mapsto \boldsymbol{U}(p)$ is weakly continuous $\rightsquigarrow$ there is a **position operator** (self-adjoint & unbounded) $\boldsymbol{Q} := -i\boldsymbol{U}'(0)$, satisfying $\boldsymbol{Q}\delta_q = q\delta_q$ in $\mathcal{D}(\boldsymbol{Q}) := \{\Psi \in \ell^2(\mathbb{R}) \, : \, \sum_{q\in\mathbb{R}} q^2|\Psi(q)|^2 < \infty\}$.

Momentum representation on $\ell^2(\mathbb{R})$

$$\boldsymbol{U}(p)\delta_{p_0} := \delta_{p_0+p}\,, \quad \boldsymbol{V}(q)\delta_{p_0} := e^{iqp_0}\delta_{p_0}\,, \quad \forall q, p, p_0 \in \mathbb{R}.$$

- $p \mapsto \boldsymbol{U}(p)$ is not weakly continuous (no position operator).
- $q \mapsto \boldsymbol{V}(q)$ is weakly continuous $\rightsquigarrow$ there is a **momentum operator** (self-adjoint & unbounded) $\boldsymbol{P} := -i\boldsymbol{V}'(0)$, satisfying $\boldsymbol{P}\delta_p = p\delta_p$ in $\mathcal{D}(\boldsymbol{P}) := \{\Psi \in \ell^2(\mathbb{R}) \, : \, \sum_{p\in\mathbb{R}} p^2|\Psi(p)|^2 < \infty\}$.

Representations of the Weyl algebra

Theorem (Halvorson, 2001)

In any representation of the CCR's in Weyl form if Q exists and has an eigenvector then P does not exist [and viceversa].

Proof: Let U_a, V_b a representation of the Weyl algebra, then, if $V_b\phi = \lambda_b\phi$, $\forall b \in \mathbb{R}$ we have $e^{iab}\langle\phi, U_a\phi\rangle = \langle\phi, U_a\phi\rangle$ and hence $\langle\phi, U_a\phi\rangle = C\delta_{0a}$ and $a \mapsto U_a$ is discontinuous.

Comments

- These representations built in $\ell^2(\mathbb{R})$ **have no analogue** in $\ell^2(\mathbb{N})$
- They were independently found and discussed by Ashtekar, Fairhurst and Willis.
- The non-existence of either momentum or position operators make it difficult to build observables of physical interest (Hamiltonians,...).
- This difficulty can be circumvented by **polymerization** (this is well known within the community, in particular by LQC practicioners.)

- Polymeric HO $\rightsquigarrow$ Toy model for LQC & LQG.
- Understand the role of **non-separability** in simple quantum mechanical systems.

To what extent the standard 1-d harmonic oscillator and the poly-harmonic oscillator are similar?

Do we recover the standard energy levels $(n+\frac{1}{2})\hbar\omega$ in an appropriate limit?

What about degeneracies? Statistical Mechanics? Physical applications?

An important comment: the spectrum for the poly-HO **cannot be a pure-point one** and **countable** because the countable set of eigenvectors cannot provide a Hilbert basis for the non-separable Hilbert space of the poly-HO (any such orthonormal basis **should be uncountable**).

Polymer Hilbert spaces

- The Hilbert spaces used to study the poly-HO, $L^2(\boldsymbol{b}\mathbb{R}, \nu_{\boldsymbol{b}\mathbb{R}})$ (the Bohr compactification of the real line) or the Hilbert space of almost periodic functions $AP(\mathbb{R}, \mathbb{C})$, are **unitarily isomorphic** to $\ell^2(\mathbb{R})$.
- The Hilbert space $AP(\mathbb{R}, \mathbb{C})$ consists of (complex) **almost periodic** functions $[f(x) = \sum_{n\in\mathbb{N}} a_n e^{i\lambda_n x},\ a_n \in \mathbb{C},\ \lambda_n \in \mathbb{R},\ \sum_{n\in\mathbb{N}} |a_n|^2 < +\infty]$.

  with scalar product $\langle \psi_1, \psi_2 \rangle_{AP} = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} \overline{\psi_1(y)} \psi_2(y)\, \mathrm{d}y\,.$
- By using appropriate linear isomorphisms (such as the Fourier-Bohr transform), both the position and the momentum representations described above can be implemented in $L^2(\boldsymbol{b}\mathbb{R}, \nu_{\boldsymbol{b}\mathbb{R}})$ or $AC(\mathbb{R}, \mathbb{C})$.
- If we use $L^2(\boldsymbol{b}\mathbb{R}, \nu_{\boldsymbol{b}\mathbb{R}})$ as the carrier of the position representation, the operator Q is a derivative operator and its square is (minus) the Laplacian $-\Delta$.
- See, for instance (Chojnacki) and references therein.

Polymerized Hamiltonians

Let $W : \mathbb{R} \to \mathbb{R}$ be a periodic piecewise continuous function. W defines, by multiplication in the algebra of almost periodic functions, a bounded operator W (potential) in $AP(\mathbb{R}, \mathbb{C})$. The operator $H = -\boldsymbol{\Delta} + W$ is self-adjoint and unbounded in an appropriate domain.

The crucial result to obtain the spectrum of H (Chojnacki):

H has only *pure point spectrum* that coincides with the spectrum of the operator $H = -\Delta + W$, with periodic potential W, defined on $L^2(\mathbb{R}, \mu_{\mathbb{R}})$.

We can then use the well-known theorems (that encapsulate the Bloch theorem of the physicists or the Floquet theory of the mathematicians) to show that the spectrum of $H = -\Delta + W$ consists of **bands**.

The eigenvalue equations (say, for the Hamiltonian) can be equivalently written as *difference equations* in $\ell^2(\mathbb{R})$ or as *differential equations* in $L^2(\boldsymbol{b}\mathbb{R}, \nu_{\boldsymbol{b}\mathbb{R}})$ or $AP(\mathbb{R}, \mathbb{C})$.

Classical Hamiltonian

$$H(q,p) = \frac{\hbar^2}{2m\ell^2}p^2 + \frac{m\ell^2\omega^2}{2}q^2\,,\ (p\,,q\ \text{dimensionless}).$$

Position representation: Introduce a length scale $q_0\ell$

$$\boldsymbol{H}(q_0) := \frac{\hbar^2}{2m(2q_0\ell)^2}\Big(2 - \boldsymbol{V}(2q_0) - \boldsymbol{V}(-2q_0)\Big) + \frac{m\ell^2\omega^2}{2}\boldsymbol{Q}^2.$$

Momentum representation: Introduce a momentum scale $p_0\hbar/\ell$

$$\boldsymbol{H}(p_0) := \frac{\hbar^2}{2m\ell^2}\boldsymbol{P}^2 + \frac{m\ell^2\omega^2}{2(2p_0)^2}\Big(2 - \boldsymbol{U}(2p_0) - \boldsymbol{U}(-2p_0)\Big).$$

By requiring $\frac{\hbar}{\ell}p_0 = m\omega q_0\ell$ the spectra coincide.

Different reps for the poly-HO

- The **eigenvalue equation** in the $\ell^2(\mathbb{R})$ position representation is

$$\frac{\hbar^2}{2m(2q_0\ell)^2}\Big(2\Psi(q)-\Psi(q+2q_0)-\Psi(q-2q_0)\Big)+\frac{m\ell^2\omega^2}{2}q^2\Psi(q)=E\Psi(q)\,,$$

with $\sum_{q\in\mathbb{R}}|\Psi(q)|^2<\infty\,,\quad \sum_{q\in\mathbb{R}}q^4|\Psi(q)|^2<\infty$, (a **difference equation**).

- The **eigenvalue equation** in $L^2(\boldsymbol{b}\mathbb{R},\nu_{\boldsymbol{b}\mathbb{R}})$ is the differential equation

$$\psi''(p)+\left(\frac{2E}{m\ell^2\omega^2}-\frac{\hbar^2}{m^2\ell^4\omega^2q_0^2}\sin^2(q_0p)\right)\psi(p)=0\,.$$

with $\psi\in L^2(\boldsymbol{b}\mathbb{R},\nu_{\boldsymbol{b}\mathbb{R}})$ in the domain of $\boldsymbol{Q}^2=-\boldsymbol{\Delta}$.

- A change of variables gives the Mathieu equation

$$\varphi''(x)+\left(\frac{E}{2m\omega^2(q_0\ell)^2}-\frac{1}{2}\left(\frac{\hbar}{2m\omega(q_0\ell)^2}\right)^2(1-\cos x)\right)\varphi(x)=0\,.$$

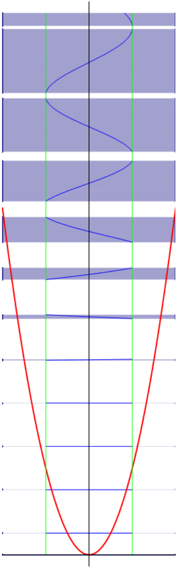
- The simplest way to model the poly-HO in the position representation is by approximating p^2 as $\boldsymbol{P}(q_0)^2 := \left(\frac{i}{2q_0}(V(q_0) - V(-q_0))\right)^2$
- There is a **huge ambiguity** here (Corichi, Vukašinac & Zapata). In the position representation on $L^2(\boldsymbol{b}\mathbb{R}, \nu_{\boldsymbol{b}\mathbb{R}})$, one can use **any** π/q_0-periodic function $W(\cdot|q_0) : \mathbb{R} \to \mathbb{R}$ such that

$$\lim_{q_0 \to 0} W(p|q_0) = \frac{\hbar^2}{m^2 \ell^4 \omega^2} p^2 \quad \text{(pointwise)}\,.$$

- A very simple such choice is the π/q_0-periodic extension of a purely quadratic (pq) potential

$$W_{\mathrm{pq}}(p|q_0) := \frac{\hbar^2}{m^2 \ell^4 \omega^2} p^2\,, \quad p \in \Big[-\frac{\pi}{2q_0}, \frac{\pi}{2q_0}\Big]\,.$$

Main features of the poly-HO spectrum



- Band structure for $H = -\Delta + W_{\rm pq}$ where $W_{\rm pq}$ is the periodic potential satisfying $W_{\rm pq}(x) = x^2$ for $x \in [-4, 4]$.
- This corresponds to choosing $q_0 = \pi/8$ and $\ell = \hbar = m = \omega = 1$.
- The plot shows the potential in one period, the bands that constitute the spectrum $\sigma(H)$, and the trace of the transfer matrix $M(E)$ that determines the position of the bands as those values of the energy for which $\mathrm{Tr}\, M(E) = \pm 2$.
- The narrow lowest energy bands closely correspond to the lowest quantum harmonic oscillator eigenvalues.

Main features of the poly-HO spectrum

It is a **band spectrum** similar to the one obtained for 1-dim periodic potentials in standard quantum mechanics formulated in separable Hilbert spaces. It is **qualitatively equal** to the one given by the Mathieu equation.

All the points in the bands are **actual eigenvalues** (i.e. are associated with "normalizable states"). Notice that the band spectrum corresponding to a periodic potential in $L^2(\mathbb{R}, \mu_{\mathbb{R}})$ is a *continuous spectrum*!

Although the lowest lying part of the spectrum of the poly-HO resembles the spectrum of the standard HO (the energies are close to the values $(n+\frac{1}{2})\hbar\omega$ in the limit when the "polymer length" goes to zero) there are some crucial differences (**infinite degeneracy**). These may be relevant:

- From the point of view of statistical mechanics (how do you define the microcanonical or canonical ensembles in this case?).
- Fock quantization of the polymerized scalar field.

Statistical mechanics: comments

Neither the **microcanonical** nor the **canonical** ensembles are well defined.

- The statistical entropy for the system as a function of the energy is

$$\Omega(E) := \mathrm{Tr}\Big(\sum_{\epsilon\in\sigma(\boldsymbol{H})\cap(-\infty,E]} \boldsymbol{P}_{\boldsymbol{H}}(\epsilon)\Big) = \sum_{\epsilon\in\sigma(\boldsymbol{H})\cap(-\infty,E]} d(\epsilon)$$

  where $d(E)$ is the degeneracy of the energy eigenvalue E. The continuous sums written above are **ill defined** owing to the uncountable number of energy eigenstates of the system.

- Likewise the canonical partition function is also ill-defined.

$$Z(\beta) = \mathrm{Tr}(e^{-\beta\boldsymbol{H}}) = \sum_{E\in\sigma(\boldsymbol{H})} d(E)e^{-\beta E} = \infty,$$

  and, hence, also the thermal density matrix $\boldsymbol{\rho} = \dfrac{e^{-\beta\boldsymbol{H}}}{\mathrm{Tr}(e^{-\beta\boldsymbol{H}})}$.

Statistical mechanics: comments

- The situation is conceptually different from the one corresponding to a standard Hamiltonian $H = -\Delta + W$ in $L^2(\mathbb{R}, \mu_{\mathbb{R}})$ for a one-dimensional periodic potential W.
- The spectrum of H is *purely absolutely continuous*, bounded from below, and the operators $e^{-\beta H}$ are trace class for $\beta > 0$.
- The **microcanonical entropy** is $\Omega(E) = \int_{\sigma(H)\cap(-\infty,E]} g(\epsilon)\mathrm{d}\epsilon$, ($g(E)$ is the density of states per energy interval).
- The **partition function** is $Z(\beta) = \int_{\sigma(H)} g(E)e^{-\beta E}\mathrm{d}E$.

We have no problem now because **there are no energy eigenvalues.**

Some comments relevant to LQG and LQC.

- The kinematical Hilbert spaces originally used in LQG are non-separable. The expectation is that **Physical Hilbert spaces are separable**.
- The polymer quantization of the parameterized scalar field (Laddha & Varadarajan) supports this view.
- Working with abstract graphs from the start may be the way to avoid non-separable kinematical Hilbert spaces in LQG (though in the end this may not even be necessary).
- **A word of caution:** It is difficult to understand how non-separable Hilbert spaces could be *Physical* Hilbert spaces. One should be very careful when using them as toy models!!
- **Superselection rules** (if applicable) may be used to avoid some problems.
- One has to find **physical criteria** to eliminate most of the eigenstates of the Hamiltonian and leave a countable number of them.

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