Observables in Quantum Mechanics and the importance of self-adjointness

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We are focused on the idea that observables in quantum physics are a bit more then just hermitian operators and that this is, in general, a "tricky business". The origin of this idea comes from the fact that there is a subtle difference between symmetric, hermitian, and self-adjoint operators which are of immense importance in formulating Quantum Mechanics. The theory of self-adjoint extensions is presented through several physical examples and a great emphasis is given on the physical implications and applications.

I. INTRODUCTION

Proper quantization of physical systems requires a correct definition of physical observables (such as the Hamiltonian, momentum, etc.) as self-adjoint operators in an appropriate Hilbert space and their spectral analysis. This problem is a much more subtle issue then the mere prescription of assigning a hermitian operator (or matrix) to a classical observable. Solution to this problem is not straightforward for nontrivial quantum systems (systems on nontrivial manifolds, in particular on manifolds with boundaries or with singular interactions). These nontrivial quantum systems with singular potentials, both relativistic and non-relativistic, with or without boundaries, play an important role in physics, and a consistent and well defined quantization requires a considerable amount of preliminary information from different advanced chapters of functional analysis. However, the content of such chapters usually goes beyond the scope of the mathematical apparatus presented in standard textbooks on Quantum Mechanics (QM) for physicists[1], e.g., [2] and even in recently published textbooks [4]. The main aim of this paper is twofold. First goal is of pedagogical nature, namely, to convince the reader-physicist that one must be very careful when reading standard textbooks on QM for physicists and particularly careful when applying the notions and prescriptions from such textbooks to nontrivial systems. The second goal is to review some of the recent (and not so recent) applications and bring the reader to the frontier of some of the latest research where the self-adjoint issues play a crucial role. The mathematical apparatus of QM is functional analysis, more specifically, the theory of linear operators in Hilbert spaces. This is a quite "subtle science" and it takes considerable time to master it. For this reason, standard textbooks on QM for physicists present a rather simplified version of the relevant parts of functional analysis in the form of brief "rules" (sometimes even called axioms[2]!) such that many mathematical subtleties are necessarily left aside or "swept under the rug". These "rules" are, more or less, based on our experience in finite-dimensional linear algebra, which often proves to be misleading and lead to some paradoxes when taken too literally. We will outline some of these paradoxes in Section II in order to motivate the reader-physicist.

Observables are usually presented as hermitian operators (matrices). Hermitian matrices have important properties like real eigenvalues, the corresponding eigenvectors are orthogonal and span the whole finite-dimensional Hilbert space, etc. However, all this properties are not ensured by the hermiticity condition in general infinite-dimensional Hilbert space. Hermiticity condition is often just replaced with the symmetricity condition, which only ensures for the expectation values of observables to be real [3], while the rest of the properties can only be grasped with imposing the more subtle condition called self-adjoitness.

A crucial subtlety is that an unbounded[3] self-adjoint (SA) operator cannot be defined in the whole Hilbert space, i.e. on an arbitrary QM state[4], which is usually assumed in a preliminary idealized scheme of operator quantization.

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[1] There are some exceptions such as [1] which are mainly intended for mathematically minded physicists and mathematicians

[2] See the Appendix A

[3] See Appendices B and C for definitions.

[4] Here "state" is used in the physical jargon and actually means an element of the Hilbert space $\mathcal{H}$(or an equivalence class of elements up to a phase). The state of a system is a positive linear map $\rho : \mathcal{H} \longrightarrow \mathcal{H}$ for which $Tr(\rho) = 0$. States can be pure or mixed. A state ρ_ψ is called pure if it maps $\psi \longmapsto \frac{(\psi,\ \cdot\ )}{(\psi,\psi)}$, $\forall \psi \in \mathcal{H}$. Thus, we can associate to each pure state ρ_ψ an element in $\mathcal{H}$. However, this correspondence is not one-to-one, and one should have this fact in mind. The physicist refer to the operators ρ as density matrices and

One must be aware that there is no operator without its domain of definition: an operator is not only a rule of acting, but also a domain in a Hilbert space to which this rule is applicable (see [3] for an elaborate discussion). In the case of unbounded operators, the same rule for different domains generates different operators with sometimes completely different properties. Provided a rule of acting is given, it is an appropriate choice of a domain for a QM observable that makes it a SA operator. The main problems and unwanted paradoxes are related to this point. But only when we understand where and why these problems occur, can we look to find ways to resolve them.

The theory of SA extensions of unbounded symmetric operators provides the main tool for solving these problems. It turns out that these extensions are generally non-unique, if they are possible at all. From the physical standpoint, this implies that when quantizing a nontrivial system, we are generally presented with different possibilities for its quantum description. The general theory describes all that mathematics can offer to a physicist. Of course, a physical interpretation of available SA extensions is a purely physical problem. Any extension is a certain prescription for the behavior of a physical system under consideration near its boundaries and singularities. We also believe that each extension can be understood through an appropriate regularization and a subsequent limit process, although this is generally a complicated problem in itself.

SA extensions are known to play important roles in a variety of physical contexts including Aharonov-Bohm effect [5, 6], two and three dimensional delta function potentials [7], anyons [8], anomalies [9], ζ-function renormalization [10], particle statistics [11], black holes [12], integrable system [13], quasinormal modes [14] and even resolving the spacetime singularities [15].

The outline of the paper is as follows. In section II, we motivate the reader by giving some paradoxes of conventional QM, and together with the appendices we establish the notation and give an overview on the formalism of QM, Hilbert spaces and properties of certain operators. In section III we give a pedagogical, step by step introduction to the subtleties of SA operators and its extensions. This is done by going through simple examples. Finally, in section IV we discuss the existence of new bound states, anomalies and give a simple proof of Pauli's theorem. The more rigorous[5] definitions and some discussions are given in the appendices in the end of the paper.

II. MOTIVATION

In order to motivate a physicist to learn about the subtleties of functional analysis we will present some paradoxes that even appear in simple QM systems[6] obtained in the idealized scheme of operator canonical quantization[7]. We show that if one follows this postulates literally, we arrive at certain paradoxes in the form of obvious contradictions with well-known statements.

Let us consider an example of a very simple system: a free non-relativistic particle of mass m moving on an interval (a, b) of the real axis. The interval can be finite or infinite, a semi-axis or the whole axis (depending on the value of a and b). The finite ends of an interval are considered to be included in the interval; in particular, by a finite interval, we mean a closed interval $[a, b]$.

In classical mechanics, the phase space $\mathcal{P} = T^*M$ of this system is a strip $(a, b) \times \mathbb{R}$; the ranges of the particle position x and momentum p are respectively (a, b) and $\mathbb{R}$. The Poisson bracket of x and p is $\{x, p\} = 1$. Free motion is defined by the free Hamiltonian $H = p^2/2m$. If $|a| < \infty$ and/or $|b| < \infty$, the peculiarity of the system is that its phase space is a space with boundaries. The behavior of the particle near the boundaries must be specified by some subsidiary conditions such as elastic/nonelastic/plastic reflection, delay, trapping or something else.

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often in Dirac notation just write $\rho = |\psi\rangle \langle\psi|$.

[5] Claims like "rigorous definition" or "rigorous proof" are also very often used in the physicist jargon. The thing is that objects are either well defined or not, or the claim is proven or not. There is no degree of "how much" something is or can be proven, but when physicist says that something is rigorously done, it just means that "all the necessary" assumptions that deal with questions of convergence, completeness, domains etc are assumed to be valid (or better say omitted). Or simply, the nonrigouros proofs or definitions seems to work well in several cases and one just takes it for granted that the results apply for other situations also.

[6] As they are usually presented on conventional undergraduate or graduate physics courses.

[7] See Appendix A for postulates of QM

At first glance, we may not face the problem of boundaries when naively quantizing this system. The canonical observables for a QM particle are the position operator $\hat{x}$ and the momentum operator $\hat{p}$ satisfying the canonical commutation relations

$$[\hat{x}, \hat{p}] = i\hbar \{x, p\} = i\hbar. \tag{1}$$

For a complete set of observables, we can take the position operator $\hat{x}$ with the prescription that its spectrum[8] be given by $\sigma(\hat{x}) = (a, b)$. It is natural to take the x-representation of canonical commutation relations where the Hilbert space $\mathcal{H}$ of states is the space of functions $\psi(x)$ square-integrable[9] on the interval (a, b); $\mathcal{H} = L^2(a, b)$; the operator $\hat{x}$ is the operator of multiplication by x, namely

$$\hat{x}\psi(x) = x\psi(x); \tag{2}$$

while the operator $\hat{p}$ is a multiple of the differentiation operator $\frac{\mathrm{d}}{\mathrm{d}x}$;

$$\hat{p} = -i\hbar \frac{\mathrm{d}}{\mathrm{d}x}, \quad \hat{p}\psi(x) = -i\hbar\psi'(x). \tag{3}$$

The canonical commutation relation obviously holds. Other observables are certain differential operators

$$\hat{f} = f(x, -i\hbar \frac{\mathrm{d}}{\mathrm{d}x}) + O(\hbar). \tag{4}$$

In particular the free quantum Hamiltonian is given by

$$\hat{H} = \frac{\hat{p}}{2m} = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2}. \tag{5}$$

All this appears quite natural from the following standpoint as well. If $|a| < \infty$ and/or $|b| < \infty$, the space $L^2(a, b)$ can be considered the subspace of functions vanishing outside the interval (a, b) in the space $L^2(\mathbb{R})$ of states of a particle on the whole axis $\mathbb{R}$, whereas all the observables defined on $L^2(a, b)$, including $\hat{x}$ and $\hat{p}$, can be considered restrictions to this subspace of well-known SA operators defined on $L^2(\mathbb{R})$. For the case of a finite interval $[a, b]$, the position operator $\hat{x}$ becomes a bounded SA operator defined everywhere [32]. Considering $\hat{p}$ as an SA operator, we have a set of three SA operators $\hat{x}$, $\hat{p}$ and $\hat{H}$ with the commutation relations

$$[\hat{x}, \hat{p}] = i\hbar, \quad [\hat{x}, \hat{H}] = 0. \tag{6}$$

If all the previous statements hold, then the following observations seem paradoxical and cast doubt on the consistency of the adopted quantization scheme.

A. Paradox 1

Let ψ_p be a normalized eigenvector of the SA operator, $\hat{p}\psi_p = p\psi_p$. Based on the self-adjointness of the operators $\hat{p}$ and $\hat{x}$, we have the following chain of equalities

$$\begin{aligned} (\psi_p, [\hat{x}, \hat{p}]\psi_p) &= (\psi_p, \hat{x}\hat{p}\psi_p) - (\psi_p, \hat{p}\hat{x}\psi_p) \\ &= p(\psi_p, \hat{x}\psi_p) - (\hat{p}\psi_p, \hat{x}\psi_p) \\ &= p\left[(\psi_p, \hat{x}\psi_p) - (\psi_p, \hat{x}\psi_p)\right] = 0, \end{aligned} \tag{7}$$

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[8] In finite dimensional space the spectrum of an operator is the set of its eigenvalues. In general Hilbert space the spectrum of a SA operator is much more. It can have point spectrum part (related to set of eigenvalues) and continuous spectrum part (usually related to generalized eigenfunctions that physicist sometimes call scattering states)[16].

[9] Here one should be aware of the full details of the construction of the Hilbert space L^2. Namely, one needs first a measurable space (M, Σ, μ) together with an equivalence relation (here M is a set, Σ is the Borel-σ-algebra and μ is a measure) $f \sim g \Leftrightarrow \|f\|_2 = \|g\|_2$ so that

$$L^2(M) := \mathcal{L}^2/\sim = \{[f] | f \in \mathcal{L}^2\}$$

where

$$\mathcal{L}^2(M, \Sigma, \mu) := \left\{ f : M \to \mathbb{C} |\ \Re(f) \text{ and } \Im(f) \text{ are measurable and } \int_M |f|^2 \, d\mu < \infty \right\}$$

with the inner product $(\cdot, \cdot) : L^2 \times L^2 \to \mathbb{C}$ and $([f], [g]) \mapsto \int_M \bar{f} g d\mu$.

which obviously contradicts the commutation relation (1), because using (1) we have

$$(\psi_p, [\hat{x}, \hat{p}]\psi_p) = i\hbar(\psi_p, \psi_p) = i\hbar \neq 0 \tag{8}$$

In addition, this commutation relations implies the well-known Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \tag{9}$$

where Δx and Δp are respective dispersion of the position and momentum for any state ψ of a particle. But for the case of a finite interval $[a, b]$ and for $\psi = \psi_p$, we have $\Delta x \leq b - a$, $\Delta p = 0$, and therefore $\Delta x \Delta p = 0$, which contradicts (9).

The explanation of the above paradoxes is different for different types of interval: depending on the type of the interval, either a SA momentum operator does not exist, or it exist but has no eigenvectors, or even if such vectors exist, they do not belong to the domain of the operator $\hat{p}\hat{x}$. In addition, in the case of a semi-axial or a finite interval, the canonical commutation relation together with the uncertainty principle do not hold. Actually the very concept of calculating commutation relations for unbounded operators is not well defined [3].

B. Paradox 2

Observe that the canonical commutation relation (1) cannot be realized for observables $\hat{x}$ and $\hat{p}$ acting as operators (matrices) on a non-trivial finite-dimensional Hilbert space $\mathcal{H}$ if the Planck's constant $\hbar$ is different from zero [35]. To see this let us assume that $\hat{x}$ and $\hat{p}$ are SA linear operators $\hat{x}, \hat{p} : \mathcal{H} \to \mathcal{H}$ such that (1) holds. Now we take the trace of (1) and calculate

$$\begin{aligned} \mathrm{Tr}([\hat{x}, \hat{p}]) &= \mathrm{Tr}(i\hbar I) \\ \mathrm{Tr}(\hat{x}\hat{p}) - \mathrm{Tr}(\hat{p}\hat{x}) &= i\hbar \mathrm{Tr}(I) \\ 0 &= i\hbar \times dim(\mathcal{H}), \end{aligned} \tag{10}$$

where we used the cyclicitiy of the trace $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$, I is the identity operator and $dim(\mathcal{H})$ is the dimension of the Hilbert space. The conclusion is that either $\hbar = 0$ or we have to abandon the idea of having a finite-dimensional Hilbert space and except the fact that at least one of the operators in question is unbounded and that the issue of trace-classness emerges also.

C. Paradox 3

We now consider a free particle moving on a finite interval $[0, a]$. If we treat a motion governed by the Hamiltonian (5) as a motion in a rectangular potential well, then the eigenvalues of the Hamiltonian and corresponding eigenfunctions are well known from any textbook:

$$\hat{H}\psi_n = E_n\psi_n, \quad E_n = \frac{\hbar^2\pi^2}{2ma}n^2, \quad \psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\Big(\frac{n\pi}{a}x\Big), \quad n \in \mathbb{N}. \tag{11}$$

The set[10] $\{\psi_n\}_1^\infty$ of these eigenfunctions is an orthonormal basis in $L^2[0, a]$, which confirms the self-adjointness of the Hamiltonian[11].

As is also well known, two commuting SA operators have common eigenvectors, and if the spectrum of the commuting SA operators are nondegenerate, then its eigenvectors must be eigenvectors of another SA operator. In our case,

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[10] $\{a_n\}_1^\infty$ denotes a set of members of the sequence a_n starting from $n = 1$ to $n = \infty$.

[11] This claim stands even rigorously, because if for a symmetric operator H its domain $D(H) \subset \mathcal{H}$ contains the orthonormal basis of $\mathcal{H}$ then H is SA (see [3]).

we have two commuting SA operators $\hat{p}$ and $\hat{H}$, and the spectrum of $\hat{H}$ is nondegenerate. Therefore, eigenfunctions of $\hat{H}$ must be eigenfunctions of $\hat{p}$. But we also have

$$\hat{p}\psi_n = -i\hbar\sqrt{\frac{2}{a}}\frac{n\pi}{a}\cos\left(\frac{n\pi}{a}x\right) \neq p_n\psi_n \tag{12}$$

for any n, which contradicts the above assertion.

This paradox is a consequence of the incorrect assumption that $\hat{p}$ and $\hat{H}$ commute; in particular, it is a consequence of the naïve belief that the Hamiltonian can be represented just as $\hat{H} = \hat{p}^2/2m$, that is as a simple composition of the operator $\hat{p}$ without refering to both of its domains.

D. Paradox 4

In standard textbooks on QM for physicists some important notions related to operators in Hilbert space are often introduced in terms of their matrix elements with respect to an orthonormal basis, because it is believed that the matrix elements $A_{mn} = (e_m, \hat{A}e_n)$ of an operator $\hat{A}$ with respect to an orthonormal basis $\{e_n\}_1^\infty$ completely determine the operator $\hat{A}$ according to the following chain of equalities:

$$\begin{gathered}\forall\psi \in \mathcal{H} \Longrightarrow \psi = \sum_{n=1}^{\infty}\psi_n e_n, \quad \psi_n = (e_n, \psi), \quad \hat{A}e_n = \sum_{m=1}^{\infty} A_{mn}e_m, \\ \hat{A}\psi = \sum_{n=1}^{\infty}\psi_n\hat{A}e_n = \sum_{m=1}^{\infty}\left(\sum_{n=1}^{\infty}A_{mn}\psi_n\right)e_m.\end{gathered} \tag{13}$$

For example, the adjoint $\hat{A}^\dagger$ of $\hat{A}$ is defined as an operator whose matrix elements are given by

$$\left(\hat{A}^\dagger\right)_{mn} = \left(e_m, \hat{A}^\dagger e_n\right) = \left(\hat{A}e_m, e_n\right) = \overline{\left(e_n, \hat{A}e_m\right)} = \overline{A_{nm}}. \tag{14}$$

Correspondingly, an SA operator $\hat{A}^\dagger = \hat{A}$ is defined as an operator whose matrix is hermitian $A_{mn} = \overline{A_{nm}}$.

But let us consider the matrix $p_{mn} = (e_n, \hat{p}e_m)$ of the momentum operator in the Hilbert space $L^2[0, l]$ with respect to the orthonormal basis $\{e_n\}_0^\infty$,

$$e_n(x) = \sqrt{\frac{2}{l}}\cos\left(\frac{n\pi}{l}x\right), \quad \forall n \in \mathbb{N}_+. \tag{15}$$

A direct calculation by integration by parts shows that

$$\overline{p_{nm}} = p_{mn} + [e_m(l)e_n(l) - e_m(0)e_n(0)] \neq p_{mn}, \quad m + n = 2k + 1, \tag{16}$$

i.e., the matrix p_{mn} is not hermitian, contrary to our expectations.

This paradox is related to the fact that the orthonormal basis (15) does not belong to the domain of any SA operator $\hat{p}$ from the whole family of admissible momentum operators. The number of these type of paradoxes can be extended [3, 16, 17, 41].

III. BASIC IDEAS AND RESULTS ON SA OPERATORS

We have seen that it is crucial to think of an operator as acting on some domain. The domain is encoded in the boundary conditions. For better understanding this issue we shall derive the basic definitions and results, which are going to be illustrated through very simple examples, step by step. The purpose of these section is to illustrate the procedure of von Neumann in simple terms using various examples from physics. Here we have mostly used [16] from which we have freely borrowed.

In order to solve a differential equation, we need to impose some boundary conditions. We know that the solution of this differential equation highly depends on these imposed boundary condition. Each boundary condition corresponds to some physically different situation, that is, nature of the interaction is encoded in the boundary condition. So, we can ask ourselves a natural question: "What are the possible choices of boundary conditions for a given operator representing an observable in QM?". Before we address this question we must remember that observables in QM must have real eigenvalues. These operators are called hermitian or SA, although as we shall see below, these two concepts are not quite the same. Having this in mind, we can thus ask the following question: "What are the possible boundary conditions that can be imposed on an operator in QM such that it is SA?". The answer to this question can be obtained from the pioneering work of von Neumann on SA extensions of operators in QM (see [16] and Appendix F).

A. Momentum operator on a line interval

To obtain the spectrum[12] of observables such as momentum or Hamiltonian in QM, we need to impose suitable boundary conditions. We shall denote a generic operator by the symbol T. The operator T acts on elements of Hilbert space $\mathcal{H}$. However, the existence of boundary conditions implies that T acts only on a subset[13] $D(T) \subset \mathcal{H}$, and not on all of $\mathcal{H}$. Elements of $D(T)$ obey the imposed boundary condition and it is clear that $D(T)$ is not the full Hilbert space $\mathcal{H}$, since there will in general be elements in $\mathcal{H}$ which would not obey the boundary condition on T. The subset $D(T)$ is called the domain of T and it is a integral part of the definition of the operator T. To illustrate this idea, let us consider the example of a momentum operator[14]

$$\hat{p} = -i\frac{\mathrm{d}}{\mathrm{d}x} \tag{17}$$

where $x \in [0,1]$. We define the domain of $\hat{p}$ as[15]

$$D(\hat{p}) = \left\{\psi(0) = \psi(1) = 0,\ \psi \text{ absolutely continuous and } \psi \in L^2[0,1]\right\}, \tag{18}$$

where $L^2[0,1]$ denotes the set of square integrable functions on the line interval $[0,1]$. Hence, the domain $D(\hat{p})$ simply encodes the boundary conditions on wavefunctions relevant for the momentum operator $\hat{p}$.

We now give a few definitions necessary for our purpose. Let the inner product of two elements $\xi, \eta \in \mathcal{H}$ be denoted by (ξ, η). An operator T is called a *symmetric operator* if the relation[16]

$$(\xi, T\eta) = (T\xi, \eta) \tag{19}$$

holds $\xi, \eta \in \mathcal{H}$. Note that this relation is sometimes used to define SA operators in elementary QM. Strictly speaking this only defines a symmetric operator and we shall see the difference between this relation and the condition for self-adjointness below.

Let $T^\dagger$ denote the operator adjoint to T. In order to fully specify $T^\dagger$, we also need to define its domain $D(T^\dagger)$. For that, let as consider a symmetric operator T and let $\xi \in D(T)$. Now find *all* elements $\eta \in \mathcal{H}$ such that

$$(\xi, T\eta) = (T\xi, \eta) \tag{20}$$

The set of all such $\eta \in \mathcal{H}$ defines[17] the *domain of the adjoint* $D(T^\dagger)$. Note that $D(T^\dagger)$ defined in this way is in general different from $D(T)$. Finally, an operator is called *self-adjoint* iff

$$T = T^\dagger, \quad D(T) = D(T^\dagger). \tag{21}$$

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[12] Physicist often thinks of the spectrum as the set of eigenvalues (point spectrum) which come from solving differential equations with certain boundary conditions and imposing square integrability of the solutions. However, to grasp the continuous part of the spectrum (or energy of the scattering states), physicist solves the same differential equation but "drops" the square-integrability condition and looks for the solution outside the Hilbert space. This at first glance strange procedure is imposed by the Dirac notation and its justification can be found in the theory of rigged Hilbert spaces (or Gelfand triples)[35][36].

[13] We also assume that $D(T)$ is dense in $\mathcal{H}$, that is $\overline{D(T)} = \mathcal{H}$ which means that the topological closure of $D(T)$ is the same as $\mathcal{H}$ ($D(T)$ may not be a complete space so dense means that the space together with limit vectors of all of its Cauchy sequences is exactly $\mathcal{H}$.)

[14] For simplicity we take the unit mass and $\hbar = 1$ system of units.

[15] From now on we understand that all derivatives are in the weak sense.

[16] This reduces to the hermicity condition in finite-dimensional Hilbert spaces.

[17] See Appendix D

Let us now illustrate the above concepts using the example of the momentum operator $\hat{p}$ with domain $D(\hat{p})$. We wish to ask the following questions:

1. Is the operator $\hat{p}$ symmetric in the given domain $D(\hat{p})$?
2. What is the domain of the adjoint $D(\hat{p}^\dagger)$?
3. Is $\hat{p}$ self-adjoint, i.e. is $D(\hat{p}) = D(\hat{p}^\dagger)$?

In order to answer this questions, consider the quantity

$$\begin{aligned}\delta_{\hat{p}} &:= (\xi, \hat{p}\eta) - (\hat{p}\xi, \eta) = -i\left(\int_0^1 \xi^* \frac{\mathrm{d}\eta}{\mathrm{d}x} - \int_0^1 \frac{\mathrm{d}\xi^*}{\mathrm{d}x}\eta\right)\mathrm{d}x \\ &= -i\left[\xi^*(1)\eta(1) - \xi^*(0)\eta(0)\right],\end{aligned} \tag{22}$$

where ξ, η at the moment are general elements of the Hilbert space $L^2[0,1]$. In order to check if $\hat{p}$ is a symmetric operator in the domain $D(\hat{p})$, consider $\xi, \eta \in D(\hat{p})$. In this case, from (18) we know $\xi(1) = \xi(0) = \eta(1) = \eta(0) = 0$. Thus we have

$$\delta_{\hat{p}} = -i\left[\xi^*(1)\eta(1) - \xi^*(0)\eta(0)\right] = 0, \quad \forall \xi, \eta \in D(\hat{p}), \tag{23}$$

which means that $\hat{p}$ is symmetric in $D(\hat{p})$.

Let us now address the second question, namely what is the domain $D(\hat{p}^\dagger)$ of the adjoint operator. For that, consider $\eta \in D(\hat{p})$ and ask what are all possible ξ such that $\delta_{\hat{p}} = 0$. Since $\eta \in D(\hat{p}), \eta(1) = \eta(0) = 0$, we see that $\delta_{\hat{p}} = 0$ is satisfied for any $\eta \in D(\hat{p})$ without any condition on ξ. This means

$$D(\hat{p}^\dagger) = \left\{\psi,\ \psi \text{ absolutely continuous and } \psi \in L^2[0,1]\right\}. \tag{24}$$

Finally we address the third question above, i.e. is $D(\hat{p}) = D(\hat{p}^\dagger)$? Comparing (18) and (24) we immediately see that the answer is *no*, as $D(\hat{p}) \subset D(\hat{p}^\dagger)$ as subsets of the Hilbert space $\mathcal{H}$. This means that the momentum operator as defined in (17) and (18) is not a SA operator! In order to further verify this statement, let us recall that if an operator is SA, then it must have a real spectrum. It is easy to verify that the eigenvalue equation

$$\hat{p}\psi = p\psi, \quad \psi(1) = \psi(0) = 0, \tag{25}$$

has no real solutions for the eigenvalue p, which is in agreement with the above observation.

The above discussion shows that the momentum operator $\hat{p}$ with the simple domain (18) is not a SA operator. This happens due to the fact that the domain of the adjoint operator turns out to be much bigger that the domain of the operator itself. The next question is whether there exists some other domain in which $\hat{p}$ is indeed self-adjoint? In order to address this question, let us consider a different domain for $\hat{p}$, namely

$$D_\theta(\hat{p}) = \left\{\psi(1) = \mathrm{e}^{\mathrm{i}\theta}\psi(0),\ \psi \text{ absolutely continuous and } \psi \in L^2[0,1]\right\}, \tag{26}$$

where $\theta \in \mathbb{R} \bmod 2\pi$. We shall also assume that $\psi(0) \neq 0$ since in that case, (26) reduces to (18). We again ask the previous three questions for the momentum operator in the domain $D_\theta(\hat{p})$.

To see if $\hat{p}$ is symmetric in $D_\theta(\hat{p})$, again consider arbitrary elements $\xi, \eta \in D_\theta(\hat{p})$. In this case,

$$\delta_{\hat{p}} = -i\left[\xi^*(1)\eta(1) - \xi^*(0)\eta(0)\right] = -i\left[\mathrm{e}^{-\mathrm{i}\theta}\xi^*(0)\mathrm{e}^{\mathrm{i}\theta}\eta(0) - \xi^*(0)\eta(0)\right] = 0, \quad \forall \xi, \eta \in D_\theta(\hat{p}). \tag{27}$$

Thus $\hat{p}$ is symmetric in $\xi, \eta \in D_\theta(\hat{p})$.

Lets us now find the domain of the adjoint in this case. As before, consider $\eta \in D_\theta(\hat{p})$ and ask what are possible ξ so that $\delta_{\hat{p}} = 0$. Since $\eta \in D_\theta(\hat{p})$, $\eta(1) = \mathrm{e}^{\mathrm{i}\theta}\eta(0)$ we see that in order to find the domain of the adjoint we have to find all $\xi \in \mathcal{H}$ by solving the equation

$$\delta_{\hat{p}} = -i\left[\xi^*(1)\eta(1) - \xi^*(0)\eta(0)\right] = 0. \tag{28}$$

This implies that

$$\eta(0)\left[\xi^*(1)\mathrm{e}^{\mathrm{i}\theta} - \xi^*(0)\right] = 0 \ \Rightarrow\ \xi(1) = \mathrm{e}^{-\mathrm{i}\theta}\xi(0) \quad \text{as} \quad \eta(0) \neq 0. \tag{29}$$

We therefore see that

$$D_\theta(\hat{p}^\dagger) = \left\{\psi(1) = \mathrm{e}^{\mathrm{i}\theta}\psi(0),\ \psi \text{ absolutely continuous and } \psi \in L^2[0,1]\right\}, \tag{30}$$

that is, $D_\theta(\hat{p}^\dagger) = D_\theta(\hat{p})$. This also answers the third question as it shows that $\hat{p}$ is indeed SA in the domain $D_\theta(\hat{p})$.

Finally, we can check that the eigenvalue equation for $\hat{p}$ in this case is given by

$$\hat{p}\psi = p\psi, \quad \psi(1) = \mathrm{e}^{\mathrm{i}\theta}\psi(0), \tag{31}$$

has the solutions

$$\psi_\theta(x) = \mathrm{e}^{\mathrm{i}px}, \quad p = 2n\pi + \theta, \tag{32}$$

where $n \in \mathbb{Z}$. It may be noted that for each value of the parameter θ, the spectrum is different. We thus have a one parameter family of inequivalent quantizations of the momentum operator on a line interval.

B. von Neumann's method of SA extension

In the previous subsection we saw that the momentum operator is not SA on the domain (18) but with a suitable choice of domain, that is (26), it can be made SA. However, the domain (26) was chosen in an ad hoc fashion, which in general is not always possible. Here, we shall discuss a method due to von Neumann which for a given operator T with a domain $D(T)$ answers the following questions:

1. Is T self-adjoint in $D(T)$?
2. If not, can it be made self-adjoint?
3. If yes, how i.e. in which domain is it self-adjoint?

In what follows, we shall not give any derivation of proofs[18] of the results but shall illustrate them with the example of the momentum operator.

We start with some definitions useful for our purpose. For a given operator T, consider equations[19]

$$T^\dagger\psi_\pm = \pm i\psi_\pm \tag{33}$$

and let $n_\pm$ denote the number of linearly independent square integrable solution of (33). The pair (n_+, n_-) are called deficiency indices for the operator T. What is their significance? Before giving a formal answer to this question note that if an operator is SA, then it is expected to have only real eigenvalues. Thus the existence of $\pm i$ in the spectrum is a measure of the deviation from self-adjointness. It is thus plausible that the deficiency indices would serve as a measure of this deviation. This idea is indeed true and any operator T can be classified in terms of its deficiency indices as follows:

1. T is (essentially) SA iff $(n_+, n_-) = (0, 0)$, or we say that it has a unique SA extension.
2. T is not SA but has SA extensions iff $n_+ = n_-$.
3. If $n_+ \neq n_-$, then T has no SA extensions.

Before we proceeding further, let us illustrate these concepts with our example of the momentum operator. Consider first the operator $\hat{p}$ with domain $D(\hat{p})$. In this case, $D(\hat{p}^\dagger)$ is given by (24). In order to find the deficiency indices, we have to solve the equations

$$-i\frac{\mathrm{d}\psi_\pm}{\mathrm{d}x} = \pm i\psi_\pm, \quad \psi_\pm(x) \in D(\hat{p}^\dagger). \tag{34}$$

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[18] For more details see [16] and Appendix E

[19] Actually we should consider $T^\dagger\psi_\pm = \pm i\kappa\psi_\pm$, where $\kappa \in \mathbb{R}$ due to dimensionality reasons (namely $[T] = [\kappa]$), but this we omit here and set $\kappa = 1$ as our "natural" choice of units. However the dimensionality of κ is very important and its physical meaning is that this is the scale of the anomaly, i.e. the breaking of the classical symmetry and it somewhat governs the physically allowed types of interaction on the boundary.

These equations have integrable solutions in the interval $[0,1]$ given by

$$\begin{aligned}\psi_+(x) &= C_+ \mathrm{e}^{-x}, \ \Rightarrow \ n_+ = 1, \\ \psi_-(x) &= C_- \mathrm{e}^{x}, \ \Rightarrow \ n_- = 1,\end{aligned} \tag{35}$$

where $C_\pm$ are normalization constants. We therefore see that in this case, $n_+ = n_- = 1$, which means that $\hat{p}$ is not SA in $D(\hat{p})$ but has SA extensions, which agrees with what we found before. What would be the deficiency indices when $\hat{p}$ is defined with the domain $D_\theta(\hat{p})$ as in (26)? In this case we have seen that $D_\theta(\hat{p}) = D_\theta(\hat{p}^\dagger)$. Hence, the deficiency indices are obtained by solving the equations

$$-i\frac{\mathrm{d}\psi_\pm}{\mathrm{d}x} = \pm i\psi_\pm, \quad \psi_\pm(1) = \mathrm{e}^{i\theta}\psi_\pm(0). \tag{36}$$

It easy to see that these equations have no square integrable solutions for real values of the parameter θ, which implies that $n_+ = n_- = 0$, i.e. $\hat{p}$ is essentially SA in $D_\theta(\hat{p})$. This too agrees with what we found before.

Let us now consider symmetric operator T in a domain $D(T)$ with deficiency indices $n_+ = n_- = n$. The above discussion tells us that T is not SA but admits SA extensions. This means that we can find a suitable domain in which T is SA. How do we find such a domain, which is necessary for calculations in QM? Here we shall again state the result[20] due to von Neumann and illustrate it with our example. For such an operator T, von Neumann's theory tells us that the domain of self-adjointness is given by[21]

$$D_U(T) = \{\psi + \psi_+ + U\psi_- |\ \psi \in D(T) \text{ and } \ U \text{ is a } \quad n \times n \text{ unitary matrix}\} \tag{37}$$

We shall now illustrate this for the case of the momentum operator $\hat{p}$. We start with the operator defined in the domain $D(\hat{p})$ as given in (18). We have seen that in this case, $n_+ = n_- = 1$ which means that it is not SA in $D(\hat{p})$. In the previous subsection we just stated what the domain of self-adjointness of $\hat{p}$ should be in an ad hoc fashion. What we shall do now is to derive the domain (26) using prescription of von Neumann.

For the case of momentum operator, let $\xi(x)$ denote an arbitrary element of the domain in (37). Our task now is to show that $\xi(x)$ constructed from the above prescription (37) obeys the boundary condition $\xi(1) = \mathrm{e}^{i\theta}\xi(0)$, where $\theta \in \mathbb{R} \bmod 2\pi$. This would illustrate the above claim about the domain of self-adjointness as we have already seen that for wavefunctions obeying such boundary conditions the momentum operator is indeed SA. In order to proceed, we first rewrite (35) with normalizations given explicitly:

$$\psi_+ = \frac{\sqrt{2}\mathrm{e}}{\sqrt{\mathrm{e}^2-1}}\mathrm{e}^{-x}, \quad \psi_- = \frac{\sqrt{2}}{\sqrt{\mathrm{e}^2-1}}\mathrm{e}^{x}. \tag{38}$$

Now note that in our case of the momentum operator, U is a 1×1 matrix, i.e. it is a phase $\mathrm{e}^{i\gamma}$, where $\gamma \in \mathbb{R}$. Now if $\xi(x)$ is an arbitrary element of the domain $D_\gamma(\hat{p})$, then from (37) we have,

$$\xi(x) = \psi(x) + \psi_+(x) + \mathrm{e}^{i\gamma}\psi_-(x), \tag{39}$$

where $\psi(x) \in D(\hat{p})$, i.e. $\psi(1) = \psi(0) = 0$ and $\psi_\pm$ are given by (38). Using this we find that

$$\begin{aligned}\xi(1) &= \psi_+(1) + \mathrm{e}^{i\gamma}\psi_-(1), \\ \xi(0) &= \psi_+(0) + \mathrm{e}^{i\gamma}\psi_-(0).\end{aligned} \tag{40}$$

Using (38) and (40) we get

$$\frac{\xi(1)}{\xi(0)} = \frac{1+\beta\mathrm{e}}{\mathrm{e}+\beta}, \quad \beta = \mathrm{e}^{i\gamma}, \quad |\beta|^2 = 1 \tag{41}$$

and taking the modulus yields

$$\left|\frac{\xi(1)}{\xi(0)}\right|^2 = 1 \ \Rightarrow \ \xi(1) = \mathrm{e}^{i\theta}\xi(0), \tag{42}$$

where $\theta \in \mathbb{R} \bmod 2\pi$. This illustrates the claim (37).

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[20] See [16] and Appendix E

[21] Here the domain is given a bit wage, since one might ask how a finite dimensional matrix U acts on ψ_-. The details are given in Appendix F, and here our wage definition is good enough since in all of our examples the matrix U will be a pure phase.

C. Free particle on a half-line

It is easy to see that the momentum operator defined on a whole half line $\mathbb{R}_+$ with the boundary condition $\psi(0) = 0$ and $\psi \in L^2(\mathbb{R}_+)$ has unequal deficiency indices. Namely, solve (33) and we get for $\psi_\pm$ exactly (35) again, but since we are looking for square integrable solution on $\mathbb{R}_+$ we get $n_+ = 1$ and $n_- = 0$. By the von Neumann theorem this implies that the momentum operator on the half line can never be realized as a SA operator in QM!

Now, let us consider the Hamiltonian for a free particle of mass $m = \frac{1}{2}$ on a half-line $x \in \mathbb{R}_+$,

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}. \tag{43}$$

Consider a subset A of the Hilbert space $\mathcal{H}$ given by

$$A = \left\{\psi \mid \psi \in L^2(\mathbb{R}_+), H\psi \in L^2(\mathbb{R}_+), \psi' \text{ absolutely continuous}\right\}. \tag{44}$$

We define the domain of the operator H as

$$D(H) = \{\psi \mid \psi \in A,\ \psi(0) = \psi'(0) = 0\}. \tag{45}$$

As before, we ask the following questions:

1. Is H symmetric in $D(H)$?
2. What is $D(H^\dagger)$
3. Is H SA in $D(H)$?

To address these issues, lets consider the expression

$$\begin{aligned}\delta_H := (\xi, H\eta) - (H\xi, \eta) &= -\int_0^\infty \left(\xi^* \frac{\mathrm{d}^2\eta}{\mathrm{d}x^2} - \frac{\mathrm{d}^2\xi}{\mathrm{d}x^2}\eta\right)\mathrm{d}x \\ &= \xi^*(0)\frac{\mathrm{d}\eta(0)}{\mathrm{d}x} - \frac{\mathrm{d}\xi^*(0)}{\mathrm{d}x}\eta(0),\end{aligned} \tag{46}$$

where ξ, η at the moment are general elements of the Hilbert space $\mathcal{H}$ which goes to zero at infinity, i.e. they are square integrable. In order to check if H is symmetric in $D(H)$, consider arbitrary $\xi, \eta \in D(H)$. In that case, from (45) we know that $\xi(0) = \xi'(0) = \eta(0) = \eta'(0) = 0$. Thus we have

$$\delta_H = \xi^*(0)\frac{\mathrm{d}\eta(0)}{\mathrm{d}x} - \frac{\mathrm{d}\xi^*(0)}{\mathrm{d}x}\eta(0) = 0, \quad \forall \xi, \eta \in D(H), \tag{47}$$

which means H is symmetric in $D(H)$.

Let us now address the second question, namely what is the domain $D(H^\dagger)$ of the adjoint operator. For that, consider $\eta \in D(H)$ and ask what are all possible ξ such that $\delta_H = 0$. Since $\eta \in D(H), \eta(0) = \eta'(0) = 0$. We thus see that $\delta_H = 0$ is satisfied for any $\eta \in D(H)$ without any condition on ξ. This means that

$$D(H^\dagger) = \{\xi \mid \xi \in A\}, \tag{48}$$

without any further condition on ξ.

Finally, we see that just as in case for the momentum operator on half-line, here also $D(H^\dagger) \supset D(H)$ as subsets of $\mathcal{H}$, and hence these two domains are not equal. This implies that H is not SA in $D(H)$.

It is now clear that the reason for the above is that the conditions defining $D(H)$ are too restrictive which leads to the condition $D(H^\dagger) \supset D(H)$. We can therefore expect that if the defining conditions on $D(H)$ are made less restrictive, i.e. if $D(H)$ is enlarged, the operator H may become SA. With that in mind, consider the following domain

$$D_\alpha(H) = \{\psi \mid \psi \in A, \psi'(0) = \alpha\psi(0)\}, \tag{49}$$

where $\alpha \in \mathbb{R}$. With this new definition of the domain, it is now easy to check that

1. H is symmetric in $D_\alpha(H)$.
2. $D_\alpha(H^\dagger) = D_\alpha(H)$.
3. Thus H is SA in $D_\alpha(H)$.

This shows that enlarging the domain of H has reduced the domain of $H^\dagger$ such that now they are equal and the operator is SA.

We shall now proceed with the method of von Neumann to analyze the operator H defined with the domain $D(H)$. In order to find the deficiency indices, we have to find square integrable solutions of the equations

$$-\frac{\mathrm{d}^2\psi_\pm}{\mathrm{d}x^2} = \pm i\psi_\pm, \quad \forall\psi_\pm \in D(H^\dagger). \tag{50}$$

The normalized solutions are

$$\begin{aligned} \psi_+ &= 2^{1/4}\exp\left(\frac{(i-1)}{\sqrt{2}}x\right), \implies n_+ = 1 \\ \psi_- &= 2^{1/4}\exp\left(\frac{-(i+1)}{\sqrt{2}}x\right), \implies n_- = 1 \end{aligned} \tag{51}$$

Following the prescription (37) of von Neumann, we can find the domain of self-adjointness of H. From (37) we expect that the SA domain of H is

$$D_\beta(H) = \{\xi \mid \xi = \psi + \psi_+ + \beta\psi_-\} \tag{52}$$

where $\psi \in D(H)$, $\psi_\pm$ are given in (51) and $\beta = \mathrm{e}^{i\gamma}$ is a unitary 1×1 matrix, i.e. a pure phase. It can be shown that if $\xi \in D_\beta(H)$, then

$$\left|\frac{\xi'(0)}{\xi(0)}\right|^2 = \frac{1-\sin\gamma}{1+\cos\gamma} \implies \xi'(0) = \alpha\xi(0) \tag{53}$$

where[22] $\alpha \in \mathbb{R}$, which is the same as the condition on the wavefunction as given by (49), i.e. the domains given by (49) and (52) are identical. Thus we again have an illustration of the prescription (37) of von Neumann. From now on, we shall no longer illustrate (37) but shall assume its validity and shall obtain the domain of self-adjointness using it as a rule. For more illustrative examples see [17].

IV. SOME PHYSICAL APPLICATIONS

A. New bound states

Let as find the solutions of the stationary Schrödinger's equation $H\psi = E\psi$ for the Hamiltonian of a free particle on a half-line given in (43)

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi, \quad \psi'(0) = \alpha\psi(0). \tag{54}$$

First consider the case when $E := k^2 > 0$. In this case the general solution is given by[23]

$$\psi = C\mathrm{e}^{-ikx} + D\mathrm{e}^{ikx}, \tag{55}$$

where C, D are constants. Imposing the boundary conditions gives

$$\frac{C}{D} = \frac{ik+\alpha}{ik-\alpha} \tag{56}$$

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[22] And the parametrization $\alpha = \pm\frac{\cos(\gamma/2+\pi/4)}{\cos(\gamma/2)}$ is used.

[23] Here one actually looks for a solution of a generalized eigenequation within the formalism of rigged Hilbert space (see Appendix F for further comments.)

which leads to the solution

$$\psi = C\left(\mathrm{e}^{-ikx} + \frac{ik+\alpha}{ik-\alpha}\mathrm{e}^{ikx}\right). \tag{57}$$

Since (57) are not elements of the Hilbert space $L^2(\mathbb{R}_+)$ we do not normalize them to 1, but rather interpret them as "stream" of particles. Therefor we have streams of particles with momentum k and $-k$ both with their corresponding amplitude. If $R := \frac{ik+\alpha}{ik-\alpha}$, we have $RR^* = 1$, i.e. $R = \mathrm{e}^{-i\theta(\alpha)}$ where $\theta(\alpha)$ is the phase of the reflected wave that depends on the parameter α. The solutions (57) represent the scattering states of the problem.

Consider next the case where $E := -\mathcal{E}$, $\mathcal{E} > 0$ and ask the question if (54) admits square integrable solutions, i.e. bound states. We try the ansatz

$$\psi = D\mathrm{e}^{\lambda x}, \quad \lambda, D \in \mathbb{R}, \tag{58}$$

From (54) with $E := -\mathcal{E}$ and (58) we have,

$$\mathcal{E} = \lambda^2 \implies \lambda_{1,2} = \pm\sqrt{\mathcal{E}} \implies \psi = D_1\mathrm{e}^{\sqrt{\mathcal{E}}x} + D_2\mathrm{e}^{-\sqrt{\mathcal{E}}x} \tag{59}$$

where $D_1 = 0$ due to square-integrability. Imposing the boundary condition on the wavefunction (59) we get,

$$\alpha = -\sqrt{\mathcal{E}} \tag{60}$$

Since $\mathcal{E} > 0$, we must have $\alpha < 0$ for square integrable bound states to exist. Thus the complete solution of the bound state eigenvalue problem is given by

$$\psi(x) = \sqrt{2\,|\alpha|}\mathrm{e}^{\alpha x}, \quad \alpha < 0, \quad E = -\alpha^2. \tag{61}$$

At this stage we pause and ask the question how is it possible for a free particle to admit a bound state. A bound state necessarily requires a scale which a free particle Hamiltonian does not contain. The answer to this apparent puzzle lies in the fact that the boundary condition (53) which defines the domain of self-adjointness supplies the necessary scale. To see this clearly, note that α in (53) has dimensions of inverse length and is the relevant dimensionful parameter related to the bound state energy. We can now go back and ask how such a dimensionfull parameter appears in the prescription of von Neumann. To understand this, note that for consistency, equations (50) for $\psi_\pm$ must have a constant with dimension length squared on the right side, whose value has conveniently been set equal to unity. Nevertheless, the dimensionfull constant actually enters the definition of the domain or equivalently the boundary condition through (50). Such a dimensionful constant breaks the scale invariance of the problem and produces the bound state when $\alpha < 0$. This is perhaps the simplest example of quantum mechanical breakdown of scale invariance, or scaling anomaly. Examples that have this exact feature are given by the δ-function potential and inverse-square potential [37].

B. Anomalies in Hamiltonian formalism

Anomalies occur when a classical symmetry is broken due to quantization [19]. In quantum field theories, anomalies were first discovered within the perturbative approach [20]. It was soon realized that anomalies are intrinsically non-perturbative in nature [21], characterized by geometric and topological structures of the theory [22]. This point of view has led to a much wider realization of anomalies in diverse areas including particle physics [23], black holes [24, 44] and important condensed matter systems such as quantum Hall systems and the associated edge states [25].

One way to understand anomalies involves the study of unbounded operators [16] in quantum theories such as the momentum and the Hamiltonian. The complete definition of such unbounded operators requires the specification of an appropriate boundary conditions or equivalently their domains so that they become SA operators. A symmetry can be implemented in the quantum theory if the corresponding generators leaves the domain of the Hamiltonian invariant and then if they commute with the Hamiltonian. Sometimes a symmetry generator does not preserve the domain of the Hamiltonian. In this case, the symmetry is broken due to quantization being thus anomalous. To see this better, let H be the Hamiltonian of some system and A a generator of symmetry. Usually in standard textbooks on QM for physicist it is stated that A is a symmetry iff $[H, A] = 0$ without any reference to the domain of operators. But the operator is defined by its rule of acting and domain. So, we have to consider operators as pairs $(H, D(H))$

and $(A, D(A))$ when evaluating the commutator, that is we have to act with the commutator on some element of Hilbert space

$$[H, A]\psi = (HA - AH)\psi = H(A\psi) - A(H\psi). \tag{62}$$

For $\psi \in D(H)$ eq. (62) makes sense only if $A\psi \in D(H)$ and $H\psi \in D(A)$. If this is not true, then anomaly appears. That is one has to check how the generator of symmetry A acts on the domain of the Hamiltonian H and see if it leaves it invariant. If yes, we say that A is a true symmetry, if not then A-symmetry is broken due to quantization and A is anomalous.

To illustrate this, let us first derive the Heisenberg equation of motion how it is usually presented in standard QM textbooks, that is by omitting the subtle domain issues. Let A be an observable represented by a SA operator, $\psi \equiv \psi(t) \in L^2(\mathbb{R})$ satisfying the Schrodinger equation

$$i\frac{\partial}{\partial t}\psi = H\psi \tag{63}$$

The expectation value of A in a state ψ is defined by

$$\langle A \rangle_\psi = (\psi, A\psi). \tag{64}$$

Now we take the time derivative $\frac{\mathrm{d}}{\mathrm{d}t}$ of (64) and using (63) we have

$$\begin{aligned}
\frac{\mathrm{d}\,\langle A \rangle_\psi}{\mathrm{d}t} &= (\frac{\partial\psi}{\partial t}, A\psi) + (\psi, \frac{\partial A}{\partial t}\psi) + (\psi, A\frac{\partial\psi}{\partial t}) \\
&= (-iH\psi, A\psi) + \left\langle \frac{\partial A}{\partial t} \right\rangle_\psi + (\psi, -iAH\psi) \\
&= \left\langle \frac{\partial A}{\partial t} \right\rangle_\psi + i(\psi, HA\psi) - i(\psi, AH\psi) \\
&= \left\langle \frac{\partial A}{\partial t} \right\rangle_\psi + i\,\langle [H, A] \rangle_\psi
\end{aligned} \tag{65}$$

which represents the Heisenberg equation of motion for the expectation values of A and often it is assumed that (65) is valid $\forall\psi \in L^2(\mathbb{R})$ so it can be written as an operator equation

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial t} + i[H, A]. \tag{66}$$

If $\frac{\mathrm{d}A}{\mathrm{d}t} = 0$ it means that $\langle A \rangle_\psi$ are constant $\forall t$ and A is called a generator of a symmetry. Often we have situations in which A does not explicitly depend on time, $\frac{\partial A}{\partial t} = 0$, so the claim $[H, A] = 0$ is equivalent to saying A generates a symmetry.

However, equation (66) and conclusions deduced from it are only valid under very strong assumptions, that were overseen in the above derivation. Namely, already in (63) one assumes $\psi \in D(H)$, in (64) $\psi \in D(A)$ is assumed, and when further calculating (65) and forming the commutator $[H, A]$ one assumes $H\psi \in D(A)$ and $A\psi \in D(H)$. Also $\psi \in D(\frac{\partial A}{\partial t})$ is assumed. Actually, the commutator $[H, A]$ and (66) is well defined only if $\psi \in \mathcal{T}$, where $\mathcal{T}$ is a subspace of $L^2(\mathbb{R})$ which is invariant under the action of H and A. Namely, $\mathcal{T}$ has to be the intersection of all the powers of H and A

$$\mathcal{T} := \bigcap_{n,m=0}^{\infty} D(H^n A^m). \tag{67}$$

$\mathcal{T}$ is called the maximal invariant subspace of the algebra generated by H and A because $A\mathcal{T}, H\mathcal{T} \subset \mathcal{T}$ and on this space all the expectation values, uncertainties etc. are well defined. Unfortunately, physicist really just need $\psi \in D(H)$ (or $\psi \in D(H) \cap D(A)$) and is interested only in solutions of (63) and therefor encounter possible problems, that is anomalies when using (65) and (66).

In order to quantify the correction to the Heisenberg equation of motion (66), let us look carefully at the second line in (65), $\frac{\mathrm{d}\langle A\rangle_\psi}{\mathrm{d}t} = \left\langle \frac{\partial A}{\partial t} \right\rangle_\psi + i(H\psi, A\psi) - i(\psi, AH\psi)$ and concentrate on the last two terms. The term $(H\psi, A\psi)$ is well defined as long as $\psi \in D(H) \cap D(A)$ while the last term $(\psi, AH\psi)$ has a problem if $H\psi \notin D(A)$. If the algebraically[24] obtained commutator $[A, H]$ is well defined on all $L^2(\mathbb{R})$ then we could write $AH = [A, H] + HA$ to obtain

$$(H\psi, A\psi) - (\psi, AH\psi) = (\psi, [H, A]\psi) - i\mathfrak{A} \tag{68}$$

where

$$\mathfrak{A} := i\left((H\psi, A\psi) - (\psi, HA\psi)\right) = i\,\langle(\,H^\dagger - H)A\rangle_\psi. \tag{69}$$

Taking the above in consideration, we can rewrite the Heisenberg equation of motion as

$$\begin{aligned} \frac{\mathrm{d}\,\langle A\rangle_\psi}{\mathrm{d}t} &= \left\langle \frac{\partial A}{\partial t} \right\rangle_\psi + i\,\langle [H, A]\rangle_\psi + \mathfrak{A} \\ \frac{\mathrm{d}A}{\mathrm{d}t} &= \frac{\partial A}{\partial t} + i[H, A] + i(H^\dagger - H)A \end{aligned} \tag{70}$$

Of course $\mathfrak{A}$ is called the anomaly [9]. We see that whenever A keeps the domain $D(H)$ invariant, $AD(H) \subset D(H)$ and $H^\dagger = H$ on $D(H)$ the anomaly vanishes $\mathfrak{A} = 0$. But whenever A does not keep the domain $D(H)$ invariant, $A\psi \notin D(H)$ the extra term in (70) will produce a non-zero surface contribution responsible for the anomaly. We can conclude the following. In the presence of the anomaly, the commutator $[H, A]$ in (66) has two contributions, the regular and anomalous part, $[H, A] = [H, A]_{reg} + [H, A]_{\mathfrak{A}}$. The regular part is the extension of the algebraically obtained commutator to the whole Hilbert space, while the anomalous part is $(H^\dagger - H)A$. It can be shown that the anomaly introduced here is equivalent to the one in the path integral approach [9, 38, 39]. This approach to anomalies [7], [9], is very general and it allows its study in a large class of quantum systems such as molecular physics [26], condensed matter systems [27], integrable models [28] and black hole physics [29]. This approach can be also adopted to quantum field theories [30], where the mode expansion encodes the information about the appropriate boundary conditions.

Here we will illustrate the occurrence of the anomaly in our simple system of non-relativistic particle on a half-line (see Section III.C and IV.A). Namely, in classical physics the Hamiltonian for our system is equal to $H = p^2$ and our system is scale invariant[25]. To put it more formally, the system is invariant under rescaling $x \longrightarrow \lambda x$ and the generator of the scale symmetry is given by the dilatation $D = tH - \frac{1}{2}xp$. It is easy to show that

$$\{H, D\} = H \tag{71}$$

which together with the Poisson bracket formalism

$$\frac{\mathrm{d}D}{\mathrm{d}t} = \frac{\partial D}{\partial t} + \{D, H\} \tag{72}$$

gives

$$\frac{\mathrm{d}D}{\mathrm{d}t} = 0, \tag{73}$$

showing that D is conserved and proving that our system is scale invariant.

Now we want to look the same system on the quantum level. Using our naive quantization procedure we would promote the classical observables H and D to operators

$$\begin{aligned} D &\longrightarrow \hat{D} = t\hat{H} - \frac{1}{4}(\hat{x}\hat{p} + \hat{p}\hat{x}) \\ H &\longrightarrow \hat{H} = \hat{p}^2 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \end{aligned} \tag{74}$$

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[24] This is usually the case, for example the canonical commutation relation $[\hat{x}, \hat{p}] = i\hbar I$, where the right hand side is algebraically obtained and as an operator is well defined on all of $L^2(\mathbb{R})$. Algebraically obtained would here mean that we calculated $[H, A]$ evaluated on $\mathcal{T}$.

[25] Actually it is $SO(2, 1)$ invariant and the symmetry is generated by the Hamiltonian H, dilatation D and conformal generator K.

and say that they act on the whole Hilbert space $L^2(\mathbb{R}_+)$ and calculate the Heisenberg equation of motion (66) and obtain

$$\frac{\mathrm{d}\hat{D}}{\mathrm{d}t} = 0, \tag{75}$$

where we used $i[\hat{D}, \hat{H}] = \hat{H}$. This way, the system would again be scale invariant and this leads to the conclusion that there cannot exist a normalizable bound state which contradicts the result found in previous subsection, namely (61). However, when deducing the non-existence of bound states we used the assumption (66) which is not valid due to domain issues of $\hat{D}$ and $\hat{H}$ and the fact that we are missing the anomaly term (69).

In section III.C we have properly defined the Hamiltonian $\hat{H}$ as a SA operator on a domain with suitable boundary conditions (53), namely $\hat{H} := (H, D_\alpha H)$ and for that operator we were able to find the bound state (61) since the new scale, the scale of symmetry breaking or anomaly came through the necessity of the parameter α which classified allowable SA boundary conditions (that is types of interaction on the boundary). Let us now calculate the anomaly (69) for our system. We have

$$\mathfrak{A} = i\left((\hat{H}\psi, \hat{D}\psi) - (\psi, \hat{H}\hat{D}\psi)\right), \quad \psi(x) = \sqrt{2\,|\alpha|}\mathrm{e}^{\alpha x}, \quad \alpha < 0. \tag{76}$$

The first term in (76) is given by

$$(\hat{H}\psi, \hat{D}\psi) = \alpha^4 t + \alpha^2(\psi, \hat{G}\psi) \tag{77}$$

where $\hat{H}\psi = -\alpha^2\psi$ and $\hat{G} = \frac{1}{4}(\hat{x}\hat{p} + \hat{p}\hat{x})$. Further

$$(\psi, \hat{G}\psi) = \frac{i\alpha}{2}\int_0^\infty dx \mathrm{e}^{\alpha x}\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}x\right)\mathrm{e}^{\alpha x} = \frac{i\alpha}{2}\int_0^\infty dx \mathrm{e}^{2\alpha x}(2\alpha x + 1) \tag{78}$$

leading to

$$(\hat{H}\psi, \hat{D}\psi) = \alpha^4 t + \frac{i\alpha^3}{2}\int_0^\infty dx \mathrm{e}^{2\alpha x}(2\alpha x + 1) \tag{79}$$

while for the second term in (76) we have

$$(\psi, \hat{H}\hat{D}\psi) = \alpha^4 t - (\psi, \hat{H}\hat{G}\psi) \tag{80}$$

where

$$(\psi, \hat{H}\hat{G}\psi) = -\frac{i\alpha}{2}\int_0^\infty dx \mathrm{e}^{\alpha x}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}x\right)\mathrm{e}^{\alpha x} = -\frac{i\alpha^3}{2}\int_0^\infty dx \mathrm{e}^{2\alpha x}(2\alpha x + 5) \tag{81}$$

leading to

$$(\psi, \hat{H}\hat{D}\psi) = \alpha^4 t + \frac{i\alpha^3}{2}\int_0^\infty dx \mathrm{e}^{2\alpha x}(2\alpha x + 5). \tag{82}$$

Combining (79), (82) and (76) we finally get

$$\mathfrak{A} = 2\alpha^3\int_0^\infty dx \mathrm{e}^{2\alpha x} = -\alpha^2 \equiv E, \tag{83}$$

so the anomaly is exactly equal to the energy of the bound state (61). Similar analysis for both the bound states and the scale anomaly can be done for the δ-function potential and $1/x^2$ potential [7, 9, 37].

C. Pauli's theorem

Pauli's theorem[26] states that time t in QM can not be a SA operator conjugate to energy E, that is it has to be regarded as an ordinary number, i.e. real parameter. The proof is analog of the statement that momentum can not

[26] For more details see [18].

be a SA operator on a half line. If we demand that the time operator $\hat{t}$ is conjugate to energy operator $\hat{E}$, then we impose the canonical commutation relation

$$[\hat{t}, \hat{E}] = i. \tag{84}$$

We can represent the operators $\hat{t}$ and $\hat{E}$ as

$$\hat{t} := i\frac{\mathrm{d}}{\mathrm{d}E}, \quad \hat{E} := E. \tag{85}$$

Since the energy of all physical systems has to be bounded from below, that is $E \in [E_0, +\infty\rangle$, we see that the deficiency indices of $\hat{t}$ are not equal[27] which implies that time cannot be realized as a SA operator conjugated to energy for systems whose energy is bounded from below.

The earliest proof, to the best of my knowledge, was given by W. Pauli [40]. He stated that since the eigenvalues for time range in $t \in \langle -\infty, +\infty\rangle$, time can not be represented as a hermitian operator (depending only on phase space variables x and p) and satisfy the commutation relation (84) since in that case energy should also range in $E \in \langle -\infty, +\infty\rangle$, which contradicts the experience, that is existence of point spectrum. He concludes that time has to be an ordinary number, a parameter in the theory.

V. QUANTUM MECHANICS IN DIMENSIONS HIGHER THEN 1

In the final section I want to point out another subtle problem of defining observables that occurs when going to dimension higher then 1. So far we have seen that in order to have well defined SA operators one needs to take care of domains. We will see that in order to pass from one dimension to two, one needs even more then just functional analysis to deal with SA, one actually needs the full machinery of differential geometry and fiber bundles [43]. However, since this goes beyond the scope of this paper I will just illustrate the problem and motivate the geometrical solution.

To this purpose let us consider QM in $d \geq 1$ dimensions. First let us define our wavefunctions as elements of a Hilbert space $\psi \in L^2(\mathbb{R}^d)$ where

$$L^2 = \mathcal{L}^2/\sim = \left\{[\psi] | \psi \in \mathcal{L}^2\right\} \tag{86}$$

and

$$\mathcal{L}^2 = \left\{\psi : \mathbb{R}^d \to \mathbb{C} |\ \Re(\psi) \text{ and } \Im(\psi) \text{ are measurable and } \int_{\mathbb{R}^d} |\psi|^2\, d^d x < \infty\right\} \tag{87}$$

with the inner product $(\cdot,\cdot) : L^2 \times L^2 \to \mathbb{C}$ and $([\psi],[\varphi]) \mapsto \int_{\mathbb{R}^d} \bar{\psi}\varphi d^d x$ that induces the equivalence relation $\psi \sim \varphi \Leftrightarrow \|\psi\| = \|\varphi\|$ and the integral is Lebesgue. In short, wavefunctions are square-integrable complex-valued functions. We will later see that exactly this has to be modified, and wavefunctions are actually sections on some appropriate bundle, but we will come to that later. Now we want to have our canonical commutation relation for coordinates q^i and momenta p_j

$$[q^i, p_j] = i\delta^i_j, \quad [q^i, q^j] = [p_i, p_j] = 0, \quad i,j = \{1, ..., d\} \tag{88}$$

and realize them as SA operators $q^i, p_j : L^2 \longrightarrow L^2$. We can represent them in the coordinate representation as multiplication operator and partial derivative respectively

$$(q^i\psi)(x) := x^i\psi(x), \quad (p_i\psi)(x) := -i\partial_i\psi(x) \tag{89}$$

and immediately we encounter various domain and target issues because if $\psi \in L^2(\mathbb{R}^d)$, because such an element ψ will either not lie in the SA domain of the operators, or the target will leave the space $L^2(\mathbb{R}^d)$. This problem

[27] Similarly as for the momentum operator on a half plane.

can be solved, as discussed in previous sections, by suitable choice of domain. Here one can construct the maximally invariant subspace $\mathcal{T} := \bigcap_{n,m=0}^{\infty} D(q^n p^m)$ which is exactly the Schwartz space[28] $\mathcal{S}(\mathbb{R}^d)$ and this resolves the domain and target issues since now $q^i, p_j : \mathcal{S}(\mathbb{R}^d) \longrightarrow \mathcal{S}(\mathbb{R}^d)$ renders the operators in question essentially SA.

The new kind of problem (that goes beyond the scope of functional analysis!) occurs if we want to switch from Cartesian to some other coordinate system. For example, let us take $d = 2$ and try to do QM in polar coordinates. Therefor we make a coordinate transformation

$$x^i \longrightarrow r, \phi, \quad p_i \longrightarrow p_r = -i\partial_r, p_\phi = -i\partial_\phi \tag{90}$$

and the commutation relations (88) still hold but we have a problem with self-adjointness (even worse, the operator p_r is not even symmetric!). It is easy to see that $x^i = \{r, \phi\}$ are symmetric, and the same hold for p_ϕ, $(\psi, p_\phi \varphi) = (p_\phi \psi, \varphi)$. But for the $p_r = -i\partial_r$ we have

$$(\psi, p_r \varphi) = -i \int r dr d\phi \bar{\psi} \partial_r \varphi = (p_r \psi, \varphi) + i \int dr d\phi \bar{\psi} \varphi \tag{91}$$

and the last term destroys the symmetry property. Therefore the quantization in coordinates other than Cartesian is not working at all. The solution to this problem is to realize that wave functions ψ are not $\mathbb{C}$-valued functions, but rather a section of a complex line bundle over[29] $\mathbb{R}^d$, that is $\psi \in \Gamma(E)$ and $E \xrightarrow{\pi_E} \mathbb{R}^d$. If so, we could improve our quantization procedure by replacing the partial derivatives ∂_i with covariant derivatives ∇_i, knowing that covariant derivative acts differently on different objects, namely

$$\begin{aligned} &\nabla_i f = \partial_i f \text{ if } f : \mathbb{R}^d \to \mathbb{C} \\ &\nabla_i \gamma = \partial_i \gamma + \omega_i \gamma \text{ if } \gamma \in \Gamma(E) \end{aligned} \tag{92}$$

where ω_i is the Yang-Mills field. Therefore, let us propose that $\psi \in \Gamma(E)$ and $p_i = -i\nabla_i$. For the Cartesian coordinates we have $\omega_i = 0$ and everything is ok. In the polar coordinates we had no problems with p_ϕ so $\omega_\phi = 0$. For $p_r = -i\nabla_r$ in order to have the symmetry property $(\psi, p_r \varphi) = (p_r \psi, \varphi)$ we get a condition on ω_r as

$$2\Re(\omega_r) = \frac{1}{r} \tag{93}$$

and it is easy to see that the canonical commutation relations still hold. Also, it is important to note, that this construction works for any dimension d, and even if we move from flat $\mathbb{R}^d$ space to same curved space, i.e. Riemann manifold (M, g). In that case, the analog analysis gives the generalization of (93) to

$$2\Re(\omega_j) = \partial_j(\log \sqrt{g}) \tag{94}$$

where g is the determinate of the metric.

This all is justified by the fact that if ψ is a section of a complex line bundle over $\mathbb{R}^d$, it locally looks like a $\mathbb{C}$-valued function. $E \xrightarrow{\pi_E} \mathbb{R}^d$ is an associated bundle to the frame bundle $LM \xrightarrow{\pi} \mathbb{R}^d$ and on a frame bundle we can establish a connection that gives rise to a covariant derivative. Also, sections of an associated bundles can be represented as $\mathbb{C}$-valued functions on the total space of the principle bundle $\psi : LM \longrightarrow \mathbb{C}$, and on the principle bundle exists an exterior covariant derivative $D\psi = d\psi + \omega\psi$. The theory of fiber bundles is one of the most important achievements in modern mathematics and it has numerous applications in various branches of mathematics and theoretical physics [45], but its immediate occurrence in QM is quite remarkable [46–49]. Here we end this work and leave further discussion and progress for another paper or lectures.

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[28] see Appendix G

[29] Or over some manifold M in general.

Appendix A: Postulates of QM

In physics, quantization means constructing a Quantum Theory (QT) for a given classical system by the so called "correspondence principle". The "correspondence principle" requires that the QT must reproduce the predictions of the initial classical theory in the classical limit(large masses, macroscopic scales, smooth potentials, and so on), which is formally the limit $\hbar \to 0$, where $\hbar$ is the Planck constant[30]. The quantization problem usually does not have a unique solution. The only criterion for whether a constructed QT is proper, is determent by the coincidence of its predictions with experiment. Experience in quantization of simplest systems (such as a free particle, a harmonic oscillator, and a non-relativistic particle in some potential fields) was used to formulate a consistent general scheme of operator quantization for an arbitrary system with canonical Hamiltonian equations of motions for phase-space variables. This scheme is called *canonical quantization*. Here, we will outline the *postulates* of *canonical quantization*[31] as they are usually expounded in standard textbooks on QM for physicists:

1. For a physical system under consideration, it is assumed that there exists a canonical Hamiltonian formulation of classical mechanics. The state of the system at any instant of time is specified by a point in some even-dimensional phase space; the points in this space are labeled by canonical generalized coordinates x_a and momenta p_a, $a = 1, ..., n$, where n is the number of degrees of freedom. The time evolution of a state of the system in the course of time t is described by the Hamiltonian equations of motion:

$$\dot{x}_a = \{x_a, H\}, \quad \dot{p}_a = \{p_a, H\}, \tag{A1}$$

where $H = H(x, p)$ is the Hamiltonian of the system and $\{,\}$ is the canonical Poisson bracket. The Poisson bracket of two arbitrary functions f and g on the phase space is defined by

$$\{f, g\} = \sum_a \left(\frac{\partial f}{\partial x_a} \frac{\partial g}{\partial p_a} - \frac{\partial f}{\partial p_a} \frac{\partial g}{\partial x_a} \right), \tag{A2}$$

in particular, we have $\{x_a, x_b\} = \{p_a, p_b\} = 0$ and $\{x_a, p_b\} = \delta_{ab}$. Classical observables (local physical quantities described by real functions of the phase-space variables) form a real associative commutative algebra.

2. In QM, a state of a physical system at any instant of time is completely specified by a vector ψ in a Hilbert space $\mathcal{H}$. A scalar product of two vectors ψ_1 and ψ_2 is denoted by (ψ_1, ψ_2). To a first approximation, it is assumed that any state $\psi \in \mathcal{H}$ can be realized physically; in particular, the superposition principle holds: if states ψ_1 and ψ_2 are realizable, then the state $\psi = a_1\psi_1 + a_2\psi_2$ with any $a_1, a_2 \in \mathbb{C}$ is also realizable.

3. In QT, each classical observable $f = f(x, p)$ is assigned a self-adjoint (SA) operator $\hat{f}$, $f \mapsto \hat{f}$, acting in Hilbert space $\mathcal{H}$. It is called a quantum observable. To a first approximation, it is assumed that any operator $\hat{f}$, including observables, is defined[32] on any state ψ, i.e., $\hat{f}\psi \in \mathcal{H}$, $\forall \psi \in \mathcal{H}$, and is uniquely determined by its matrix elements $(\psi_1, \hat{f}\psi_2)$, $\forall \psi_1\psi_2 \in \mathcal{H}$, and what is more, by its matrix $f_{mn} = (e_m, \hat{f}e_n)$ with respect to any orthonormal basis[33] $\{e_n\}_1^\infty$, a complete orthonormalized set of vectors in $\mathcal{H}$. Then any operator $\hat{f}$ is assigned its adjoint $\hat{f}^\dagger$ defined by

$$\left(\psi_1, \hat{f}^\dagger\psi_2\right) = \left(\hat{f}^\dagger\psi_1, \psi_2\right), \quad \forall \psi_1, \psi_2 \in \mathcal{H}, \tag{A3}$$

and thereby the involution (conjugation) $\hat{f} \mapsto \hat{f}^\dagger$ is defined in the algebra of operators with the properties[34]

$$\begin{aligned} &\left(\hat{f}^\dagger\right)^\dagger = \hat{f}, \quad \left(a\hat{f}\right)^\dagger = \bar{a}\hat{f}^\dagger, \quad \forall a \in \mathbb{C} \\ &\left(\hat{f} + \hat{g}\right)^\dagger = \hat{f}^\dagger + \hat{g}^\dagger, \quad \left(\hat{f}\hat{g}\right)^\dagger = \hat{g}^\dagger\hat{f}^\dagger. \end{aligned} \tag{A4}$$

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[30] In mathematics, quantization is a quantum deformation of classical structures; the deformation parameter is the Planck constant $\hbar$.

[31] There are mainly three well established formulation of QM: 1. Heisenberg's matrix mechanics (historically first, but of less practicable use for a working physicist); Scrödinger's wave mechanics (standard and most used formalism); Feynman's path integral (wildly used in relativistic quantum field theories). Actually, in general, one can formulated consistent non-relativistic QM in (at least) nine independent ways [31]

[32] To be precise this only holds for finite-dimensional Hilbert spaces and for bounded operators in infinite-dimensional Hilbert spaces. In physics we are usually dealing with unbounded operators, for which every operator has its domain.

[33] $\{\psi_n\}_1^\infty$ is an infinite sequence of vectors.

[34] The bar $^-$ over an expression denotes complex conjugation

The self-adjointness[35] of $\hat{f}$ means $\hat{f} = \hat{f}^\dagger$, or

$$\left(\psi_1, \hat{f}\psi_2\right) = \left(\hat{f}\psi_1, \psi_2\right), \quad \forall \psi_1, \psi_2 \in \mathcal{H} \tag{A5}$$

The mean value $\left\langle \hat{f} \right\rangle_\psi$ of any quantum observable $\hat{f}$ in a state ψ and the corresponding dispersion Δf are respectively defined by

$$\left\langle \hat{f} \right\rangle_\psi = \frac{\left(\psi, \hat{f}\psi\right)}{(\psi, \psi)}, \quad \Delta f = \sqrt{\left\langle \hat{f}^2 \right\rangle_\psi - \left\langle \hat{f} \right\rangle_\psi^2}. \tag{A6}$$

The self-adjointness of observables is assumed to imply that any observable $\hat{f}$ can be diagonalized, which means that the eigenvectors, or eigenstates, of $\hat{f}$ form an orthonormal basis in $\mathcal{H}$; the spectrum of an observable is defined as a set of all its eigenvalues. The spectrum determines possible measurable values of the corresponding observable, while the complete orthonormalized set of the eigenstates of the observable provides a probabilistic interpretation of its measurements.

4. According to the correspondence principle, there exists a certain relation between the Poisson bracket of classical observables and the commutator $[,]$ of their quantum counterparts. Namely,

$$\{f_1, f_2\} \to \frac{1}{i\hbar}\left[\hat{f}_1, \hat{f}_2\right] + \hat{O}(\hbar) \tag{A7}$$

The position operators $\hat{x}_a$ and momentum operators $\hat{p}_a$ are postulated to be SA and satisfy the canonical commutation relations

$$[\hat{x}_a, \hat{x}_b] = [\hat{p}_a, \hat{p}_b] = 0, \quad [\hat{x}_a, p_b] = i\hbar\{x_a, p_b\} = i\hbar\delta_{ab} \tag{A8}$$

The correspondence principle requires that the quantum counterpart $\hat{f}$ of a classical observable $f(x,p)$ be of the form $\hat{f} = f(\hat{x}, \hat{p}) + \hat{O}(\hbar)$. A supplementary operator $\hat{O}(\hbar)$ is generally necessary to provide the self-adjointness of $\hat{f}$. In the general case, the correspondence principle does not allow a unique construction of the operator function $f(\hat{x}, \hat{p})$ in terms of the classical function $f(x,p)$ because of the noncommutativity of $\hat{x}$ and $\hat{p}$ (the so-called ordering problem[36]). To the first approximation whereby any observable can be diagonalized, it is argued that commuting observables $\hat{f}_1$ and $\hat{f}_2$ have a joint spectrum, i.e., a common set of eigenvectors, which implies the simultaneous measurability of the observables. A complete set of observables is defined as a minimum set of n commuting observables $\hat{f}_k$, $k = 1, ..., n$, $[\hat{f}_k, \hat{f}_l] = 0$, $\forall k, l$ whose joint spectrum is nondegenerate and whose common eigenvectors provide a unique specification of any vector in terms of the corresponding expansion with respect to these eigenvectors. Different complete sets of observables can be considered, and their spectrum and eigenvectors specify the quantum description of a system under consideration.

5. The time evolution of a state of the system in the course of time t is described by the Schrödinger equation for the state vector $\psi(t)$,

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi, \tag{A9}$$

with an initial condition $\psi(t_0) = \psi_0$, where the operator $\hat{H}$, the quantum Hamiltonian, the energy observable, corresponds to the classical Hamiltonian H.

Appendix B: Bounded linear operators

Let $(\mathcal{V}, \|\cdot\|_\mathcal{V})$ be a normed space and $(\mathcal{W}, \|\cdot\|_\mathcal{W})$ a Banach space[37]. A linear map $T : \mathcal{V} \longrightarrow \mathcal{W}$ is called a bounded linear operator if

$$\sup_{f \in \mathcal{V}\setminus\{0\}} \frac{\|Tf\|_\mathcal{W}}{\|f\|_\mathcal{V}} < \infty \tag{B1}$$

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[35] More precisely see Appendix C.
[36] A substantial contribution to the resolution of this problem is due to Berezin [34]
[37] A Banach space is a normed and complete space (all Cauchy sequences are convergent in it).

For a bounded operator one can define the so called operator norm $\|\cdot\|$ such that

$$\|T\| = \sup_{f\in\mathcal{V}\setminus\{0\}} \frac{\|Tf\|_{\mathcal{W}}}{\|f\|_{\mathcal{V}}} \tag{B2}$$

and there are theorems that state that a linear map is continuous[38] if and only if this map is a bounded operator and that a bounded operator is defined on all of $\mathcal{V}$, that is $D(T) = \mathcal{V}$. For these operators the naive quantization prescription would work much better, but unfortunately (or fortunately!) in physics we almost always have to deal with observables that are unbounded (the operator norm is ill-defined), like the paradoxes in section II illustrate. Also note that a Hilbert space is always a Banach space since the inner product $(\cdot,\cdot)_{\mathcal{H}}$ induces a norm $\|\cdot\|_{\mathcal{H}} = \sqrt{(\cdot,\cdot)_{\mathcal{H}}}$.

Appendix C: Hilbert spaces

In this appendix, we remind the reader of basic notions and facts from the theory of Hilbert spaces.

- A Hilbert space $\mathcal{H}$ is a linear space over the complex numbers. As a rule, the elements of $\mathcal{H}$ (vectors or points) are denoted by Greek letters: $\xi, \eta, \zeta, \psi, ... \in \mathcal{H}$ whereas numbers, complex or real, are denoted by italic Latin letters: $a, b, c, x, y, z, ... \in \mathbb{C}$ or $\mathbb{R}$. In what follows , we consider infinite-dimensional Hilbert spaces.

- The space $\mathcal{H}$ is endowed with a scalar product that is a positive definite sesquilinear form on $\mathcal{H}$. This means that every pair of vectors ξ, η is assigned a complex number (ξ, η), the scalar product of ξ and η, with the properties

$$\begin{aligned} &(\xi,\eta) = \overline{(\eta,\xi)}; \quad (\xi,\xi) \geq 0, \quad \text{and} \quad (\xi,\xi) = 0 \iff \xi = 0; \\ &(\xi, a\zeta + b\eta) = a(\xi,\zeta) + b(\xi,\eta) \Rightarrow (a\xi + b\zeta, \eta) = \bar{a}(\xi,\eta) + \bar{b}(\zeta,\eta). \end{aligned} \tag{C1}$$

  The nonnegative arithmetic square root $\sqrt{(\xi,\xi)}$ is called the norm, or length, of a vector ξ, and is denoted by $||\xi|| = \sqrt{(\xi,\xi)}$. A vector ξ is called normalized if $||\xi|| = 1$. Any nonzero vector ξ can be normalized: $\xi \mapsto \xi^n = \xi/||\xi||$. For any two vectors ξ and η, the *Cauchy-Schwarz-Bunyakovskii inequality* $|(\xi,\eta)| \leq ||\xi||\,||\eta||$ holds. A corollary of the Cauchy-Schwarz-Bunyakovskii inequality is the triangle inequality $||\xi+\eta|| \leq ||\xi|| + ||\eta||$ for the norm. The distance between two points ξ and η is defined as $||\xi - \eta||$. The triangle inequality for the distance becomes $||\xi-\eta|| \leq ||\xi-\zeta|| + ||\eta-\zeta||$. The distance determines the topology[39] in $\mathcal{H}$. A sequence $\{\xi_n\}_1^\infty$ of vectors is said to be convergent to a vector ξ, or equivalently, we say that ξ is the limit of this sequence, written $\xi_n \to \xi$, $n \to \infty$, or $\xi = \lim_{n\to\infty}\xi_n$, if $||\xi_n - \xi|| \to 0$, $n \to \infty$. Because of the triangle inequality, a necessary condition for convergence is

$$||\xi_m - \xi_n|| \to 0, \quad m, n \to \infty. \tag{C2}$$

  A sequence $\{\xi_n\}_1^\infty$ with property (C2) is called a fundamental sequence or a Cauchy sequence. Linear operations in $\mathcal{H}$ (multiplication of vectors by complex numbers and vector addition) and the scalar product are continuous in their arguments; for example,

$$\xi_n \to \xi \Rightarrow (\xi_n, \eta) \to (\xi, \eta), \quad \forall \eta \in \mathcal{H}. \tag{C3}$$

  because of the Cauchy-Schwarz-Bunyakovskii inequality. A set $M \subset \mathcal{H}$ is said to be dense in $\mathcal{H}$ if any vector in $\mathcal{H}$ can be approximated by vectors belonging to M with any desired accuracy, i.e., if for any $\xi \in \mathcal{H}$, there exists a sequence $\{\xi_n\}_1^\infty$, $\xi_n \in M$, so that $\xi = \lim_{n\to\infty}\xi_n$.

- $\mathcal{H}$ is complete. This means that every Cauchy sequence $\{\xi_n\}_1^\infty$ in $\mathcal{H}$ is convergent, or has a limit in $\mathcal{H}$:

$$||\xi_m - \xi_n|| \to 0, \quad m, n \to \infty \quad \Rightarrow \quad \exists \xi \in \mathcal{H} : \xi_n \to \xi, \quad n \to \infty. \tag{C4}$$

  As mentioned above, any convergent sequence $\{\xi_n\}_1^\infty$ is a Cauchy sequence. In a Hilbert space, the converse also holds[40]. A space that satisfies the first two requirements is called a pre-Hilbert space. Any pre-Hilbert space can be made a complete Hilbert space by adding the "limits" of Cauchy sequences. Note that the requirement of completeness is crucial, and not only technical, for applications of Hilbert spaces to QM.

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[38] with respect to the topologies induced by the respective norms on $\mathcal{V}$ and $\mathcal{W}$

[39] A Hilbert space is a particular case of a normed and metric space in which a norm and a metric (distance) satisfying standard requirements are generated by a scalar product; see [33]

[40] In short, a Hilbert space is complete with respect to a metric generated by a scalar product.

- A Hilbert space $\mathcal{H}$ is called separable if it contains a countable dense set. Separable Hilbert spaces are sufficient for treating conventional QM.
- The Hilbert space $L^2(a,b)$ is the linear space of square-integrable functions on an interval (a,b) of the real axis,

$$L^2(a,b) = \left\{ \psi(x) : \int_a^b \mathrm{d}x \ |\psi(x)|^2 < \infty \right\}. \tag{C5}$$

The scalar product in $L^2(a,b)$ is defined by

$$(\psi_1, \psi_2) = \int_a^b \mathrm{d}x \ \overline{\psi_1}(x)\psi_2(x). \tag{C6}$$

It is significant that the integral are Lebesgue integrals, and strictly speaking, the elements of $L^2(a,b)$ are equivalence classes of functions that are equal almost everywhere[41].

Appendix D: Adjoint of an operator and its properties

Definition. The adjoint $A^\dagger$ of a densely defined linear operator $A : D(A) \longrightarrow \mathcal{H}$ is defined by

1. $D(A^\dagger) := \{\psi \in \mathcal{H} | \exists \eta \in \mathcal{H} : \forall \alpha \in D(A) : (\psi, A\alpha) = (\eta, \alpha)\}$
2. $A^\dagger \psi = \eta$

Definition. A densely defined[42] linear operator $A : D(A) \longrightarrow \mathcal{H}$ is called symmetric if $\forall \alpha, \beta \in D(A) : (\alpha, A\beta) = (A\alpha, \beta)$.

Lemma. If A is symmetric, then $A \subseteq A^\dagger$ meaning

1. $D(A) \subseteq D(A^\dagger)$
2. $A^\dagger \psi = A\psi, \quad \forall \psi \in D(A)$

Appendix E: Self-adjoint operators and their properties

Definition. A densely defined operator $\hat{f}$ is called a *self-adjoint operator (SA operator)* if it coincides with its adjoint, $\hat{f} = \hat{f}^\dagger$. In the language of maps, this means that $\hat{f}$ is symmetric, and $D_f = D_{f^\dagger}$.

Lemma. A *symmetric operator* $\hat{f}$ is SA iff $\xi_* \in D_{f^\dagger} \Rightarrow \xi_* \in D_f$, i.e.,

$$\left(\xi_*, \hat{f}\xi\right) = \left(\hat{f}^\dagger \xi_*, \xi\right), \quad \forall \xi \in D_f \Rightarrow \xi_* \in D_f \tag{E1}$$

To make sure that an operator $\hat{f}$ is SA, we can verify that 1. $\hat{f}$ is symmetric and that 2. the criterion of the above Lemma holds.

It is not infrequent that physicist easily verifies 1., but forgets about 2., which must never be forgotten. Physical QM observables must be represented by SA operators, and not simply symmetric ones. Only SA operators possess the remarkable properties of a real-valued spectrum and a complete orthogonal system of (in general "generalized") eigenvectors corresponding to this spectrum, which provides the possibility of a probabilistic physical interpretation of QM states, observables, and measurements.

Lemma. All means of an SA operator $\hat{f}$ are real, $(\xi, \hat{f}\xi) = \overline{(\xi, \hat{f}\xi)}$, $\forall \xi \in \quad D_f$, and determine the norm of the operator,

$$\left\| \hat{f} \right\| = \sup_{\xi \in D_f, ||\xi||=1} \left| (\xi, \hat{f}\xi) \right|. \tag{E2}$$

Lemma. The following relations hold for SA operators:

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[41] When speaking about some function belonging to $L^2(a,b)$ and possessing some additional specific properties like absolute continuity, we actually mean the representative of the corresponding equivalence class.

[42] Densely defined means that the domain D_f is dense in $\mathcal{H}$, i.e. $\overline{D_f} = \mathcal{H}$

1. $\hat{f} = \hat{f}^\dagger, a \in \mathbb{R} \Rightarrow a\hat{f} = (a\hat{f})^\dagger, D_{af} = D_f$.

2. $\hat{f} = \hat{f}^\dagger, \hat{g} = \hat{g}^\dagger, \overline{D_f \cap D_g} = \mathcal{H} \Rightarrow (\hat{f} + \hat{g})^\dagger \supseteq \hat{f} + \hat{g}$. In general, the sum $\hat{f} + \hat{g}$ of two SA operators is no more than symmetric if densely defined, but if one of the operators, let it be $\hat{g}$, is defined everywhere, and is therefore bounded, then the sum is an SA operator, $\hat{f} + \hat{g} = (\hat{f} + \hat{g})^\dagger$ with $D_{f+g} = D_f$.

3. $\hat{f} = \hat{f}^\dagger, \hat{g} = \hat{g}^\dagger, \overline{D_{fg}} = \mathcal{H} \Rightarrow (\hat{f}\hat{g})^\dagger \supseteq \hat{g}\hat{f}$. In general, the product $\hat{f}\hat{g}$ of two SA operators is not even symmetric; the product $\hat{f}\hat{g}$ is symmetric, $(\hat{f}\hat{g})^\dagger \supseteq \hat{f}\hat{g}$, if $\hat{f}$ is defined everywhere, and therefore bounded, and if $\hat{g}\hat{f} \subseteq \hat{f}\hat{g}$, i.e., $\hat{f}$ and $\hat{g}$ commute; the product $\hat{f}\hat{g}$ is SA, $(\hat{f}\hat{g})^\dagger = \hat{f}\hat{g}$, if both $\hat{f}$ and $\hat{g}$ are defined everywhere, and are therefore bounded, and commute, $[\hat{f}, \hat{g}] = 0$.

The property 2. is of particular importance for physics. If the unbounded SA "free" Hamiltonian $\hat{H}_0$ is perturbed by a bounded SA potential $\hat{V}$ defined everywhere, then the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ is SA with $D_H = D_{H_0}$. But if $\hat{V}$ is unbounded, then the sum $\hat{H}_0 + \hat{V}$ in general is no more than symmetric if densely defined, and we encounter the problem of its SA extension.

In contrast to the general unbounded operators, SA operators allow one to define the notion of their commutativity, which can be done in terms of the one-parameter family $\left\{\hat{U}_f(\alpha) = \exp(\mathrm{i}\alpha\hat{f}), \alpha \in \mathbb{R}\right\}$ of mutually commuting unitary operators[43]

$$\left[\hat{U}_f(\alpha), \hat{U}_f(\beta)\right] = 0, \forall\alpha, \beta \in \mathbb{R}, \tag{E3}$$

associated with each SA operator $\hat{f}$. Self-adjoint operators $\hat{f}$ and $\hat{g}$ are called commuting, or commute, if the respective families $\left\{\hat{U}_f(\alpha)\right\}$ and $\left\{\hat{U}_g(\alpha)\right\}$ of the associated unitary operators mutually commute: $\left[\hat{U}_f(\alpha), \hat{U}_g(\beta)\right] = 0, \forall\alpha, \beta \in \mathbb{R}$.

The families of associated unitary operators make it possible to formulate some nontrivial commutation relations for SA operators. For example, the canonical commutation relation $[\hat{q}, \hat{p}] = i\hbar$ for the position operator $\hat{q}$ and the momentum operator $\hat{p}$ is properly formulated as the Weil relation [32]

$$\hat{U}_q(\alpha)\hat{U}_p(\beta) = \mathrm{e}^{-\mathrm{i}\alpha\beta}\hat{U}_p(\beta)\hat{U}_q(\alpha), \quad \forall\alpha, \beta \in \mathbb{R}, \tag{E4}$$

for the corresponding associated unitary operators $\hat{U}_q(\alpha) = \exp(\mathrm{i}\alpha\kappa_0\hat{q})$ and $\hat{U}_p(\beta) = \exp(\mathrm{i}\beta\hat{p}/\kappa_0\hbar)$, where κ_0 is a fixed parameter of dimension of inverse length.

Appendix F: The von-Neumanns theorems

The first von Neumann theorem

For any symmetric operator $\hat{f}$, the domain $D_{f^\dagger}$ of its adjoint $\hat{f}^\dagger$ is the direct sum of the three subspaces[44] $D_{\bar{f}}, \Sigma_{\bar{z}}$ and Σ_z:

$$D_{f^\dagger} = D_{\bar{f}} + \Sigma_{\bar{z}} + \Sigma_z, \quad \forall z \in \mathbb{C}', \tag{F1}$$

such that any vector $\xi_* \in D_{f^\dagger}$ is uniquely represented as

$$\xi_* = \underline{\xi} + \xi_z + \xi_{\bar{z}}, \quad \underline{\xi} \in D_{\bar{f}}, \quad \xi_z \in \Sigma_{\bar{z}}, \quad \xi_{\bar{z}} \in \Sigma_z, \tag{F2}$$

which is called the *first von Neumann formula* and

$$\hat{f}^\dagger\xi_* = \overline{\hat{f}}\underline{\xi} + z\xi_z + \bar{z}\xi_{\bar{z}}. \tag{F3}$$

The second von Neumann theorem

A symmetric operator $\hat{f}$ is essentially SA iff its deficiency indices[45] are equal to zero, $m_\pm = 0$. A symmetric operator

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[43] Note that unitary operators are bounded and defined everywhere, and the notion of commutativity for such operators is unambiguous.

[44] Where $\mathbb{C}'$ is a set of complex numbers with nonzero imaginary part, $\mathbb{C}' = \{z = x + iy, y \neq 0\} = \mathbb{C}_+ \cup \mathbb{C}_-$. If we define $\hat{f}(z) = \hat{f} - z\hat{I}$, then $\Sigma_z = \ker\hat{f}^\dagger(\bar{z}) = \left\{\xi_{\bar{z}} \in D_{f^\dagger} : \hat{f}^\dagger\xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}\right\}$ and $\Sigma_{\bar{z}} = \ker\hat{f}^\dagger(z) = \left\{\xi_z \in D_{f^\dagger} : \hat{f}^\dagger\xi_z = z\xi_z\right\}$

[45] Deficiency index is defined as $m(z) = \dim\ker\hat{f}^\dagger(\bar{z}) = \{m_+, \text{ for } z \in \mathbb{C}_+ \text{ or } m_- \text{for } z \in \mathbb{C}_-\}$

$\hat{f}$ is essentially maximal, i.e., does not allow nontrivial symmetric, much less SA, extensions iff one of its deficiency indices is equal to zero, $\min m_\pm = 0$, while the other is nonzero, $\max m_\pm \neq 0$. If $\min m_\pm = 0$, i.e., both deficient subspaces $\Sigma_{\bar{z}}$ and Σ_z of a symmetric operator $\hat{f}$ are nonzero, then nontrivial symmetric extension of $\hat{f}$ exist. Any symmetric extension $\hat{f}_U$ of $\hat{f}$ is determined by some isometric operator $\hat{U}$ with domain $D_U \subseteq \Sigma_{\bar{z}}$ and range $\hat{U}D_U \subseteq \Sigma_z$. This extension is given by

$$\begin{aligned} D_{f_U} &= D_{\underline{f}} + (\hat{I} + \hat{U})D_U \\ &= \left\{\xi_U : \xi_U = \underline{\xi} + \xi_{z,U} + \hat{U}\xi_{z,U}; \forall \underline{\xi} \in D_{\bar{f}}, \forall \xi_{z,U} \in D_U \subseteq \Sigma_{\bar{z}}; \hat{U}\xi_{z,U} \in \hat{U}D_U \subseteq \Sigma_z\right\}, \end{aligned} \tag{F4}$$

and

$$\hat{f}_U \xi_U = \overline{\hat{f}}\underline{\xi} + z\xi_{z,U} + \bar{z}\hat{U}\xi_{z,U}. \tag{F5}$$

Conversely, any isometric operator $\hat{U} : \Sigma_{\bar{z}} \to \Sigma_z$ with domain $D_U \subseteq \Sigma_{\bar{z}}$ and range $\hat{U}D_U \subseteq \Sigma_z$ defines a symmetric extensions $\hat{f}_U$ of $\hat{f}$ given by (F4) and (F5). The equality

$$\xi_U = \underline{\xi} + \xi_{z,U} + \hat{U}\xi_{z,U} \tag{F6}$$

in (F4) is called the *second von Neumann formula*.

The main theorem

Let $\hat{f}$ be an initial symmetric operator with domain D_f and adjoint $\hat{f}^\dagger$, $\hat{f} \subseteq \hat{f}^\dagger$, let $\Sigma_{\bar{z}}$ and Σ_z be the deficient subspaces of $\hat{f}$,

$$\Sigma_z = \ker \hat{f}^\dagger(\bar{z}) = \left\{\xi_{\bar{z}} : \hat{f}^\dagger \xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}\right\}, \quad \Sigma_{\bar{z}} = \ker \hat{f}^\dagger(z) = \left\{\xi_z : \hat{f}^\dagger \xi_z = z\xi_z\right\}, \tag{F7}$$

where $z \in \mathbb{C}_+$ is arbitrary, but fixed, and let $m_\pm$ be the deficiency indices of $\hat{f}$, $m_+ = \dim\Sigma_{\bar{z}}$ and $m_- = \dim\Sigma_z$. The operator $\hat{f}$ has SA extensions $\hat{f}_U = \hat{f}_U^\dagger$, $\hat{f} \subseteq \hat{f}_U$ iff both its deficient subspaces $\Sigma_{\bar{z}}$ and Σ_z are isomorphic, or iff its deficiency indices are equal, $m_\pm = m$. If the deficient subspaces are trivial, i.e., if both deficiency indices are equal to zero, $m_\pm = 0$, the operator $\hat{f}$ is essentially SA, and its SA extension is its closure $\overline{\hat{f}} = (\hat{f}^\dagger)^\dagger$, which coincides with its adjoint, $\overline{\hat{f}} = (\overline{\hat{f}})^\dagger = \hat{f}^\dagger$. If its deficient subspaces are nontrivial, i.e., if the deficiency indices are different from zero, $m_\pm = m \neq 0$, there exists an m^2-parameter family $\left\{\hat{f}_U\right\}$ of SA extensions that is the manifold $U(m)$, a unitary group. Each SA extension $\hat{f}_U$ is determined by an isometric mapping $\hat{U} : \Sigma_{\bar{z}} \to \Sigma_z$ of one of the deficient subspaces onto another and is given by

$$\begin{aligned} D_{f_U} &= D_{\overline{f}} + (\hat{I} + \hat{U})\Sigma_{\bar{z}} \\ &= \left\{\xi_U : \xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z,\ \forall \underline{\xi} \in D_{\bar{f}},\ \forall \xi_z \in \Sigma_{\bar{z}},\ \hat{U}\xi_z \in \Sigma_z\right\}, \end{aligned} \tag{F8}$$

where $D_{\overline{f}}$ is the domain of the closure $\overline{\hat{f}}$, and

$$\hat{f}_U \xi_U = \overline{\hat{f}}\underline{\xi} + z\xi_z + \bar{z}\hat{U}\xi_z. \tag{F9}$$

Conversely, any isometry $\hat{U} : \Sigma_{\bar{z}} \longmapsto \Sigma_z$ that establishes an isomorphism between the deficient subspaces defines an SA extension $\hat{f}_U$ of $\hat{f}$ given by (F8) and (F9). If the deficient subspaces are finite-dimensional, $0 < m < \infty$, then SA extensions $\hat{f}_U$ can be specified in terms of unitary matrices $U \in U(m)$. Namely, let $\{e_{z,k}\}_1^m$ and $\{e_{\bar{z}}, l\}_1^m$ be some orthogonal bases in the respective deficient subspaces $\Sigma_{\bar{z}}$ and Σ_z. Then an SA extension $\hat{f}_U$ is given by

$$\hat{f}_U : \begin{cases} D_{f_U} = \begin{cases} \xi_U : \xi_U = \underline{\xi} + \sum_{k=1}^m c_k e_{U,k},\ \forall \underline{\xi} \in D_{\overline{f}}, \\ \forall c_k \in \mathbb{C}, e_{U,k} = e_{z,k} + \sum_{l=1}^m U_{lk} e_{\bar{z},l}, \end{cases} \\ \hat{f}_U \xi_U = \overline{\hat{f}}\underline{\xi} + \sum_{k=1}^m c_k \left(z e_{z,k} + \bar{z} \sum_{l=1}^m U_{lk} e_{\bar{z},l}\right), \end{cases}, \tag{F10}$$

where $U = ||U_{lk}||$ is a unitary matrix.

Appendix G: Some basics of rigged Hilbert space

In order to find the full spectrum of an observable by solving a differential equation one needs to so called rigged Hilbert space [35, 36]. Namely, if one wants to find the full spectrum of the Hamiltonian by solving the Schrödinger equation

$$H\psi = E\psi \tag{G1}$$

then for the continuous E, one needs to "look" for solutions outside the Hilbert space $L^2(\mathbb{R})$, since the solutions in $L^2(\mathbb{R})$ exist only for discrete E (point spectrum). The basic idea of the rigged Hilbert space is to find solutions to (G1) that don't lie in $L^2(\mathbb{R})$, but rather in the adjoint of a densely defined subspace called the Schwartz space $\mathcal{S}(\mathbb{R})$. This was one constructs a Gelfand triple

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R}) \subset \mathcal{S}'(\mathbb{R}). \tag{G2}$$

The Schwartz space $\mathcal{S}(\mathbb{R})$ is the function space of all functions whose derivatives (multiplied by any monomial x^α) are rapidly decreasing (often called test functions), while $\mathcal{S}'(\mathbb{R})$ is the dual of $\mathcal{S}(\mathbb{R})$, namely the space of all continuous linear functionals $\mathcal{S}'(\mathbb{R}) : \mathcal{S}(\mathbb{R}) \longrightarrow \mathbb{C}$ (often called distributions or generalized functions).

Note that a rigged Hilbert space is not an extension of physics or QM, but rather the most natural mathematical structure required to study QM. Rigged Hilbert space is actually the equipping of a Hilbert space with the theory of distribution, and provides the full mathematical foundation for the so-called Dirac's bra-ket notation and well known Dirac's δ-function [41, 42]. In Dirac's notation the ket's $|\psi\rangle$ are elements of $\mathcal{S}(\mathbb{R})$, while the bra's $\langle\psi|$ are elements of the dual $\mathcal{S}'(\mathbb{R})$.

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