Impenetrable barriers and canonical quantization

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We address an apparent conflict between the traditional canonical quantization framework of quantum theory and spatially restricted quantum dynamics when the translation invariance of an otherwise free quantum system is broken by boundary conditions. By considering the example of a particle in an infinite well, we analyze spectral problems for related confined and global observables. In particular, we show how we can interpret various operators related to trapped particles by not ignoring the rest of the real line that is never occupied by a particle.

I. INTRODUCTION

A proliferation of papers on the pedagogical and more formal aspects of the most idealized trapping model, the infinite potential well,[1–8] sophisticated exercises in exact quantization on a half-line,[9] and the quantum mechanical approach to particles on surfaces with obstacles,[10] motivates renewed interest in reconciling the principles of canonical quantization with the analysis of well posed, spectral problems for the Hamilton operator with Dirichlet boundary conditions.

The purely spectroscopic analysis is represented in the literature on mesoscopic systems such as quantum billiards or microwave cavities.[11–13] In this analysis one avoids using canonical quantization and instead focuses on the statistical properties of the related Laplace operator eigenvalues. Issues such as the position and momentum observables and the indeterminacy relations are omitted from the analysis of these spatially trapped quantum systems.

A major surprise in this context is that a careful analysis of the conceptual background reveals unexpected inconsistencies and paradoxes.[5–8] They appear when one applies the traditional apparatus of canonical quantization to models of trapping and arise from attempts to give a correct meaning to the differential expression $-i\hbar d/dx$. It is possible to define different self-adjoint operators by means of the same differential expression that leads to conflicting options (compare Refs. 5,7,8 and Refs. 3,14,15) for what should be the momentum observable and consequently the momentum representation of wave functions for a particle in the infinite well.

The textbook canonical quantization procedure for a particle in one spatial dimension is carried out in the Hilbert space $L^2(R)$ of square integrable functions on the real line R. The canonical position and momentum operators $(Xf)(x) = xf(x)$, $(Pg)(x) = -i\hbar \frac{d}{dx} g(x)$ are defined to act on appropriate sets of functions $f, g \in L^2(R)$. If the motion of the particle remains confined to a segment $[a, b] \subset R$, then the corresponding wave functions are supported by $[a, b]$ and thus form a subspace of $L^2(R)$. This subspace may be identified with $L^2([a, b])$, the Hilbert space of square integrable functions on $[a, b]$.

Therefore, for spatially confined dynamics, it appears natural to neglect the (irrelevant) complement $R \setminus (a, b)$ of the segment $[a, b]$ and to adopt the quantization in the interval strategy.[5,7,8] One still employs the operator $-i\hbar d/dx$, but its domain is required to belong to $L^2([a, b])$; a and b are the boundary points of the well. Then, the resulting "momentum observable" has a discrete spectrum and the momentum space formulation is given in terms of a Fourier series.[5]

Although we arrive at the one-parameter family of momentum-like operators, the problem is that none of them is compatible with the infinite well (Dirichlet) boundary conditions. There is no self-adjoint operator acting as $-i\hbar d/dx$ in the subspace of wave functions in $L^2([a, b])$ which vanish at the endpoints of the interval.

On the other hand, we should notice that the canonical operators X and P are defined in $L^2(R)$ without any reference to the dynamics. Therefore, as a matter of principle, they retain their physical meaning for any conceivable motion of a particle, including the permanent trapping conditions. Implicitly, this viewpoint is represented in Refs. 14, 3, 15, and 16, where $-i\hbar d/dx$ is interpreted in $L^2(R)$ and is not confined to the interval $[a, b] \subset R$. Therefore the exterior of the infinite well does matter. The traditional momentum-space formulation for wave packets, introduced by the Fourier transform

$$\phi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \exp\left(-\frac{ipx}{\hbar}\right) \psi(x, t) dx, \tag{1}$$

has been exploited in the analysis of the infinite well and half-line versions of the wave packet dynamics.[3,14,15] The notion of a standard momentum observable with a continuous spectrum also is present in the derivation of so-called entropic uncertainty relations for the infinite well.[16]

The problem is that the differential expression $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$, whose domain contains functions $f \in L^2(R)$ such that $f(x) = 0$ if $x \leq a$ and $x \geq b$, is not a self-adjoint operator in $L^2(R)$. Hence, the infinite well energy observable definition is defective, if naively extended to $L^2(R)$ to conform with the presumed domain properties of X and P.

The above mathematical inconsistencies are normally ignored in the physics oriented literature and the primitive (infinite well) example of the quantum mechanical energy spectrum is not at all analyzed in terms of the full-fledged canonical quantization formalism. Interestingly, there is also no agreement among mathematically oriented physicists whether one can introduce a physically justified candidate for the momentum operator in the infinite well or the half-line settings. The folk lore statement reads: there is *no* momentum observable.[5]

For the above reasons we reconsider the problem of the quantum dynamics of a particle that is restricted to a segment of a line by means of impenetrable barriers. Quantum dynamics with barriers involves a number of mathematical subtleties: it is necessary to keep in mind the distinction between symmetric (Hermitian) and self-adjoint operators. A discussion of self-adjoint extensions of symmetric operators, with a focus on the teaching of quantum mechanics, can be found in Ref. 5. Our goal is to resolve the apparent momentum observable paradoxes[5,7] that prohibit a consistent use of canonical quantization procedures in the analysis of quantum systems with trapping boundary conditions.

We resolve the paradox by acknowledging the existence of the rest of the real line, in conformity with the Fourier transform definition of Eq. (1), even if we know that the trapped particle will never occupy that space. The major localization mechanism is rooted in the dynamics of the particle which is generated by a properly defined Hamiltonian.

We give physical motivations for the validity of the standard momentum observable notion for the trapped particle by investigating the infinite well as the limit of a series of finite wells. The idealization of an infinite well is given physical meaning by assuming that it approximately describes more realistic finite well models. To this end we need to maintain consistent interpretations of the concepts of position, momentum, and energy operators in the course of the limiting procedure. This consistency can be achieved if we consider the infinite well eigenfunctions as the functions in $L^2(R)$, that is, defined on the whole of R, but supported only by $[a, b] \in R$. We discuss the related energy observable issue in Secs. III, IV, and VB. We employ the usual notions of position and momentum on R and no recourse to momentum-like operators with a discrete spectrum is necessary.[5,7]

The structure of the paper is as follows. In Sec. II we outline the paradoxes that have been found to hamper a consistent discussion of quantum systems with rigid walls. In Sec. III we describe the outcome of a rigorous quantization of particle motion in a finite interval on the line R. In Sec. IV we analyze an infinite well as a limit of a finite one and discuss the groundwork for Sec. V where we propose to relax the assumptions of Sec. III (quantum mechanics in a trap only) by considering the trap exterior as a necessary element of the theory. In view of the existence of the standard notions of the position and momentum observables in $L^2(R)$, the canonical quantization procedure in the presence of impenetrable barriers is justified and removes the conceptual obstacles discussed in Sec. II.

II. QUANTUM SYSTEMS WITH BARRIERS – MATHEMATICS VERSUS PHYSICS

Although it is generally accepted that physics is written in the language of mathematics, there are disagreements on how much mathematical background is needed to give a proper description of physical phenomena.

The foundations of quantum mechanics employ both the precision of modern mathematical language and intuition based on the analysis of physical phenomena. The major developments in quantum theory and its ability to successfully describe the microworld are due more to physical intuition than to the precision of mathematics. This success is one reason why many physicists neglect sophisticated mathematical arguments.

Although we can regard the correspondence between observables and self-adjoint operators in Hilbert space as generally accepted, the precise formulation of the operator domains often is considered an unnecessary nuisance or mathematical pedantry. However, we argue that the domain subtleties in the operator analysis carry crucial physical information and must not be disregarded.

The infinite well is a special case of the class of quantum billiards, which are models of a quantum particle that is permanently trapped in a bounded region of arbitrary shape. Their energy spectra can be established only for relatively planar (R^2) confinement regions and suffer from the same momentum observable "paradoxes" as the infinite well model. Investigations of the eigenvalue problem for the Laplacian on a connected and compact domain of arbitrary shape in R^2 with Dirichlet boundary conditions have a long history.

In its full generality it is one of the most difficult problems in mathematics,[17] but suitably simplified it is a playground for the study of mesoscopic systems, quantum dots, and other nanostructures.

For a wide class of Hamiltonians, such as those with bounded potentials, one observes dispersion of wave packets. Thus, even if the particle is initially confined within a certain interval on R, there is a nonvanishing probability current through the interval boundaries.

We are interested in the situation when the quantum dynamics is so restrictive that a particle once localized cannot be found on certain parts of the real line at any time. This situation amounts to saying that there is no tunneling,[18,19] or any other form of quantum mechanical transport between those parts and their complement on R. Simple examples of such circumstances are provided by introducing impenetrable walls. These walls can be interpreted as ideal trapping enclosures on R. Typical barriers are externally imposed through suitable, often discontinuous and more singular, potentials. Less spectacular but important examples of impenetrability are related to the existence of nodes, nodal curves or surfaces of the generalized ground state function (see Refs. 18 and 19).

The notion of impenetrability does not directly follow from the canonical quantization procedure. A typical quantization recipe first presumes that there should be primitive kinematic observables related to the position and momentum, for example, the self-adjoint position and momentum operators. It is the (secondary) dynamical observable, the Hamiltonian of the system, that determines the evolution for the system. Then $\psi(x,t)$ ultimately appears as a solution of the partial differential equation with suitable initial/boundary conditions. Hence, localization essentially arises due to the dynamics with confining boundary conditions.

Observables are represented by self-adjoint operators which may be bounded or unbounded. Obviously, the generator of unitary dynamics, the Hamiltonian, has to be among them. The self-adjointness property is required because of the spectral theorem which, as a general solution of the eigenvalue problem for a given operator, determines a unique link between a operator and its family of spectral projections. The projection operators in turn let us state unambiguous elementary (yes-no) questions about the properties of a physical system. For example, by using projection operators we may ask for the probability of locating a particle in a given interval or to find its momentum within a certain range.

However, in connection with the notion of an unbounded observable, there are associated very rigid domain restrictions. We shall address this point in some detail in Sec. III. An immediate problem can be seen if we consider a particle on R and assume that it permanently resides between two impenetrable barriers (rigid walls), placed at points a and b in R. Clearly, the condition $\psi(x,t) = 0$ for all $x \leq a$ and $x \geq b$ is enforced on the wave function of a particle.

One may think that a Hamiltonian can be simply defined as as the differential operator $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$, both inside and outside the impenetrable walls. The point is that such an apparently natural, globally defined Hamiltonian is not a self-adjoint operator. It is not even a symmetric operator.[20] Hence, a consistent definition of the quantum dynamics in the presence of a barrier needs a careful examination of self-adjoint operator candidates for the Hamiltonian of the quantum system.

Another obvious conflict with intuition appears when one tries to interpret the differential expression $-i\hbar d/dx$ as a momentum operator in the barrier context. The continuous spectrum of the momentum operator for a free quantum particle on a line is well known. The notion of momentum is not so obvious for the infinite well model in view of the textbook wisdom: "…momentum operator eigenfunctions do not exist in a box with rigid walls, because then they would vanish everywhere."[21] In contrast, another well known textbook[14] does not prohibit such notions as the momentum measurement and the distribution of continuous momentum values in stationary states, these being interpreted as $L^2(R)$ wave packets. A quantum particle in an infinite well gives rise to a pictorial illustration of the wave packet dynamics.[14,15]

An attentive reader must be confused, because both discussions seem to be justified,[14,21] although the discrepancies between the two points of view were not explained or resolved in a single text. In Refs. 14, 3, and 15, an explicit answer was formulated for the probability of a measurement of the momentum P of the particle yielding a result between p and $p + dp$ for a particle confined in an infinite well. All calculations explicitly involve the $L^2(R)$ Fourier integral Eq. (1) for spatially confined wave packets, thus suggesting that the infinite well problem may not be in conflict with the standard notion of the momentum operator (understood as the generator of spatial translations in $L^2(R)$). Such an operator has a continuous spectrum.

The same infinite well problem has been summarized in Ref. 7 as follows: the spectrum of the operator P is discrete, hence the Hilbert space in the momentum representation becomes the Hilbert space l^2 of square summable sequences, see for example, Sec. III. Then, Eq. (1) is interpreted as a mathematically equivalent version of the infinite well wave function $\psi(x,t)$, but *not* as its momentum representation.

In Refs. 14, 3, and 15, the differential expression $-i\hbar d/dx$ is interpreted in $L^2(R)$, hence the exterior of the infinite well does matter. In Ref. 7, the same differential expression is localized to the interior of the well by demanding that its domain belongs to $L^2([a,b])$,with a and b the well boundaries, so the rest of the line is irrelevant.

Analogous conflicting interpretations can be seen in the discussion of a single impenetrable barrier that divides R into two non-communicating segments, see for example, Refs. 5 and 15. A quantum particle, once initially localized on the half-line, either positive or negative, would reside on the half-line indefinitely, with no chance to change the localization area. Again, the usual momentum representation[3,14,15] makes sense in the analysis of the dynamical behavior of wave packets. However, it is well known[22] that a symmetric operator $-i\hbar\frac{\partial}{\partial x}$, as defined on $C_0^\infty(R^\pm)$ (the space of the infinitely differentiable functions of compact support in the positive R^+ or negative R^- half-lines of R), has no self-adjoint extensions in $L^2(R^+)$ or $L^2(R^-)$. In other words there is no self-adjoint momentum operator of the form $-i\hbar\frac{\partial}{\partial x}$ for a particle on a half-line. Accordingly, the authors of Ref. 5 conclude that "…the momentum is not a measurable quantity in that situation."

To summarize, the standard Fourier integral analysis on the real line, Eq. (1), has been applied to wave packets of a particle confined to a segment of R or to the half-line and interpreted as a consistent spectral analysis of the momentum operator.[3,14,15] According to Refs. 5 and 7, the previous analysis can be seen only as an admissible computational device having nothing to do with the momentum operator and the true physically relevant state of affairs for a particle confined to the segment is said to refer to the spectral analysis of the momentum operator in terms of Fourier series. For a particle confined to the half-line, the notion of momentum is said not to be defined.

III. QUANTIZATION IN THE FINITE INTERVAL

We now discuss the mathematical issues of the quantization on the interval (a particle confined to a segment of R). We begin with some observations concerning a free particle on the real line R.

In one-dimensional models on the real line, the momentum operator P and the free Hamiltonian H are self-adjoint operators defined by $-i\hbar d/dx$ and $(-\hbar^2/2m)d^2/dx^2$ respectively. However, these standard differential expressions, when defined on the space $C_0^\infty(R)$ of infinitely differentiable functions of compact support, are not self-adjoint but only symmetric operators. In the following, all coefficients such as $\hbar$ and $\hbar^2/2m$ will be set equal to unity for convenience.

Because $C_0^\infty(R)$ is invariant under differentiation, the symmetric operator $-\frac{d^2}{dx^2}$ can be interpreted as the square of another symmetric operator $-i\frac{d}{dx}$, in the sense that it means two consecutive actions. To obtain the self-adjoint operators from the symmetric ones, we must expand their domains. There are a priori two possibilities:

(i) We can extend the symmetric operator $-i\frac{d}{dx}$ by taking its closure to a self-adjoint operator P, which is then called a momentum operator, and define the free particle Hamiltonian operator $H_f = P^2$.

(ii) We can extend the symmetric operator $-\frac{d^2}{dx^2}$ by taking its closure to a self-adjoint operator $\tilde{H}_f$ which may be called the Hamiltonian operator.

These two procedures give the same result: $H_f = P^2 = \tilde{H}_f$ if considered in $L^2(R)$.

The situation is different when we pass to $L^2([a,b])$, because now the mathematical subtleties unavoidably enter. It turns out that there is not one, but a family of infinitely many self-adjoint operators in $L^2([a,b])$ whose action on functions from the domain is defined by the same expression $-i\frac{d}{dx}$. In the following, we shall simplify the notation by choosing $a = 0$, $b = \pi$ and hence the Hilbert space $L^2([0,\pi])$.

The differential expressions $-i\frac{d}{dx}$ and $-\frac{d^2}{dx^2}$ when acting in $C_0^\infty(0,\pi)$ (infinitely differentiable functions with support included in the open interval $(0,\pi) \subset R$) define symmetric operators in $L^2([0,\pi])$. Obviously, $C_0^\infty(0,\pi)$ is invariant under differentiation and thus $-\frac{d^2}{dx^2}$ is the square of $-i\frac{d}{dx}$ in the sense of two consecutive actions. However, now the procedures (i) and (ii) require some care. In what follows we shall refer to the Krein-von Neumann theory of self-adjoint extensions, see for example Refs. 5, 23, and the Appendix.

Let us begin with procedure (i). We denote $A = -i\frac{d}{dx}$ on $C_0^\infty(0,\pi)$. Then its closure $\overline{A} = -i\frac{d}{dx}$ is defined as the differential expression $-i\frac{d}{dx}$ acting on an expanded domain $D(\overline{A}) = \{f \in AC[0,\pi]; f(0) = 0 = f(\pi)\}$. The notation AC refers to the absolute continuity of f which gives meaning to the first derivative f'. The boundary conditions emerge in the process of taking the closure.

The operator $\overline{A}$ is a closed symmetric operator, but is not self-adjoint. To find the self-adjoint extension of $\overline{A}$, we need to establish its deficiency indices.[5,22,23] In the Appendix we show them to be $(1,1)$, which implies that $\overline{A}$ has a one parameter family of self-adjoint extensions in $L^2([0,\pi])$. We denote the extensions by P_α:

$$P_\alpha = -i\frac{d}{dx} \quad D(P_\alpha) = \{f \in AC[0,\pi]; f(0) = \exp(i\alpha)f(\pi)\} \qquad (0 \leq \alpha < 2\pi). \tag{2}$$

Note that there are no other self-adjoint extensions of $\overline{A}$, and thus no other self-adjoint operators acting as $-i\frac{d}{dx}$. For each α, there is in $L^2([0,\pi])$ an orthonormal basis that is composed of the eigenvectors of P_α,

$$e_n^\alpha(x) = \frac{1}{\sqrt{\pi}} \exp i(2n + \frac{\alpha}{\pi})x, \tag{3}$$

where n takes integer values, and the eigenvalues of P_α are

$$p_n^\alpha = 2n + \frac{\alpha}{\pi}. \tag{4}$$

Let us introduce another definition for $D(P_\alpha)$. If $f \in L^2([0,\pi])$ is expressed in terms of e_n^α so that $f(x) = \sum_n f_n^\alpha e_n^\alpha(x)$, then $f \in D(P_\alpha)$ if and only if $\sum_n n^2 |f_n^\alpha|^2 < \infty$. This supplementary characterization of the domain will prove useful to define functions of the operators P_α, c.f. the spectral theorem description in the Appendix.

The operator H_α defined by

$$H_\alpha = (P_\alpha)^2, \tag{5}$$

has the same family of eigenvectors as P_α, but its eigenvalues are

$$E_n^\alpha = (p_n^\alpha)^2 = (2n + \frac{\alpha}{\pi})^2 \tag{6}$$

for all integers n. As a consequence,

$$D(H_\alpha) = \{f = \sum_n f_n^\alpha e_n^\alpha; \sum_n n^4 |f_n^\alpha|^2 < \infty\}. \tag{7}$$

Thus $D(H_\alpha) \subset D(P_\alpha)$ and $D(P_\alpha) = P_\alpha D(H_\alpha)$. It also follows that

$$H_\alpha = -\frac{d^2}{dx^2} \quad D(H_\alpha) = \{f \in AC^2[0,\pi]; f(0) = \exp(i\alpha)f(\pi), f'(0) = \exp(i\alpha)f'(\pi)\}, \tag{8}$$

where the AC^2 notation gives meaning to the second derivative of f. Therefore the operator H_α in Eq. (8) can be safely interpreted as two consecutive actions of P_α, Eqs. (2) and (5), where both operators are self-adjoint.

Now let us consider (ii). The closure of $-\frac{d^2}{dx^2}$ as defined on $C_0^\infty(0,\pi)$ is $\overline{H} = -\frac{d^2}{dx^2}$ with the domain $D(\overline{H}) = \{f \in AC^2[0,\pi]; f(0) = f(\pi) = f'(0) = f'(\pi) = 0\}$. The closed symmetric operator $\overline{H}$ has the deficiency indices $(2,2)$. Therefore the family of all self-adjoint extensions of $\overline{H}$ is in one-to-one correspondence with $U(2)$, the family of all 2×2 unitary matrices, see for example, Refs. 5 and 23.

We can devise a family of $U_\alpha \in U(2)$, $0 \le \alpha < 2\pi$, whose choice is equivalent to the boundary conditions $f(0) = \exp(i\alpha)f(\pi)$, $f'(0) = \exp(i\alpha)f'(\pi)$, and thus defines $H_{U_\alpha} = H_\alpha$, Eq. (5), with the domain $D(H_\alpha)$, Eq. (8). Consequently, the two procedures (i) and (ii), are equivalent for all operator pairs H_α, P_α with $0 \le \alpha < 2\pi$.

The family U_α is a proper subset of $U(2)$ and thus there are H_U for which (i) does not work. For example, for a suitable choice of a unitary matrix U,[5] the corresponding self-adjoint operator $H_U \doteq H_w$ is the infinite well Hamiltonian:

$$(H_w f)(x) = -\frac{d^2}{dx^2} f(x) \quad D(H_w) = \{f \in AC^2[0,\pi]; f(0) = f(\pi) = 0\}. \tag{9}$$

In the infinite well context provided by Eq. (9), we are not allowed to interpret H_w as the square of any self-adjoint $-i\frac{d}{dx} = P_\alpha$. The reason is that no P_α respects the Dirichlet boundary condition, which makes it impossible to identify the Hamiltonian H_w in $L^2([0,\pi])$ as P_α^2. Consequently, the quantization in a finite interval gives rise to:

(i) The one-parameter family of Hamiltonians H_α of Eq. (8) with the momentum operators P_α of Eq. (5), whose eigenvalues form discrete spectra,

(ii) The Hamiltonian H_w of Eq. (9), suitable for the infinite well problem, but then with no notion of a momentum observable.

To complete the quantization scheme on the interval, we need to introduce the position operator Q defined as $(Qf)(x) = xf(x)$. In the present case it is a bounded operator, contrary to what is normally expected from a member of a canonically conjugate position-momentum pair.

The canonical commutation relations $QP_\alpha - P_\alpha Q = iI$ formally hold on all $f \in AC(a,b)$; $f(a) = f(b) = 0$, but cannot be given in Weyl form (that is, in terms of suitable unitary operators) which is indispensable for the mathematical consistency of the canonical formalism. Note that by following the procedure (i), which yields Eq. (5), we have lost a direct link to the infinite well problem.

For the special case of $\alpha = 0$, we end up with a degenerate spectrum $E_n = (2n)^2$. This spectrum corresponds to the familiar plane rotator. For $\alpha \neq 0$, we can relate the spectral problem Eq. (6) to the rotation of a charged particle around an infinitely thin solenoid;[24] the parameter α is related to the magnetic flux. Hence, H_α, P_α refer exclusively to rotational (angular dynamics) features of motion. Neither $\frac{d^2}{dx^2}$ with the Dirichlet boundary condition, nor any other H_U (provided $U \neq U_\alpha$) fit the above canonical quantization picture; we recall that no self-adjoint momentum operator of the form $-i\frac{d}{dx}$ is compatible with the Dirichlet boundary conditions.

In connection with Eq. (6), the textbook solution of the infinite well yields the familiar spectral formula $E_n = n^2$, where $n \geq 1$ is a natural number. This result is incompatible with $E_n^\alpha = (2n + \frac{\alpha}{\pi})^2$, Eq. (6) where n is an integer. Moreover, the related eigenfunctions $e_n^\alpha(x)$, do not respect the Dirichlet boundary conditions in contrast to the "true" infinite well Hamiltonian eigenfunctions $\psi_n(x) = \sqrt{\frac{2}{\pi}} \sin nx$. A possible physical interpretation of H_U that falls neither in the class (8) nor (9) is discussed in Ref. 5.

We stress that the interpretation of P_α in Eq. (2) as a momentum operator for a trapped particle (as advocated in Refs. 5–7) stems from the fact that its differential expression reads $-i\frac{d}{dx}$, just as it does for a particle on the real line. Some obvious consequences of this implicit $L^2(R)$ input in the isolated trap, $L^2([a, b])$, include: (1) the non-uniqueness of the momentum operator, (2) the non-existence of the momentum operator on the half-line, and (3) a conceptual discontinuity in the interpretation of the momentum observable between $L^2(R)$ and $L^2([a, b])$ $L^2([a, \infty])$.[5] The latter conceptual discontinuity relates to the limiting procedures when passing from regular (such as the finite well with its unique momentum observable) to singular problems (such as the infinite well, or half-line cases, with non-unique or no momentum observable).

IV. THE INFINITE WELL AS THE LIMIT OF THE FINITE ONES

It is common for physicists to replace a complicated physical system by a simpler solvable model and then obtain approximate answers to the originally posed questions. Often the solvable models are more singular than the realistic ones. In quantum mechanics textbooks, the piecewise constant potentials that form sharp barriers, steps or wells are implicitly interpreted as idealized versions of continuous potentials of similar shapes. A more singular example is the Dirac delta potential which often is used instead of a very narrow and very deep potential well.[18,27]

Infinite well (or infinite barrier) models make sense if they are capable of giving approximate answers to questions concerning finite wells. It is important that the validity of the approximation be controlled, which requires the notion of continuity when passing from the finite well to the infinite one. In this section, we are motivated by the considerations of Ref. 5 where the previously mentioned conceptual discontinuity between the finite well and infinite well models is clearly emphasized.

It is natural to consider the half-line case as the limit of the step potential. Again we encounter problems with the idea of the momentum observable: for any finite height of the step potential, there exists a momentum observable (a unique self-adjoint operator acting as the differential expression $-i\hbar\frac{d}{dx}$), while for an infinite height there is no self-adjoint extension corresponding to $-i\hbar\frac{d}{dx}$. The conclusion of Ref. 5 (see Sec. 7.4), that "an infinite potential cannot be simply described by the limit of a finite one" contributes to the paradoxes and inconsistencies we discussed in Sec. II.

If one tries to model a particle that is localized on a segment of a line, the confinement is enforced by considering Hamiltonians with vanishing boundary conditions at the ends of the interval. This boundary condition can be imposed either by the singularity of the potential (such as the Pöschl-Teller potential in Ref. 7) or "by hand" as for the infinite well.[5,7] The latter case is justified by introducing the vague concept of a finite potential within the spatial segment and plus infinity otherwise.

The reasoning goes as follows. A particle that is trapped inside the infinite well $0 \leq x \leq \pi$ must have its wave function equal to zero outside the well. To ensure this condition, we consider the potential $V(x) = \infty$ on the complement of the open interval $(0, \pi)$ in R, while $V(x) = 0$ between the impenetrable barriers.

Note that the corresponding stationary Schrödinger equation,

$$[-\nabla^2 + V(x)]\psi(x) = E\psi(x), \tag{10}$$

with $x \in R$ has no meaning beyond the chosen interval.

By formally setting $\infty \times 0 = 0$ in the "improper" area, one argues that in view of Eq. (10), the wave function $\psi(x)$ must vanish for $x \leq 0$ and $x \geq \pi$. Then, one concludes that instead of demanding unusual properties of $V(x)$, it is more natural to impose restrictions on the wave functions demanding that $\psi \in L^2([0,\pi])$; $\psi(0) = \psi(\pi) = 0$ (the dynamics is spatially restricted to $[0,\pi]$). In other words, the rest of the line can be neglected.

Now, let us consider a (dis)continuity in passing to the infinite well from a finite well. We have mentioned that the infinite well problem acquires a physical meaning as an approximation (by suitable limiting procedures) of a finite well model. Let us consider[5] $V(x) = 0$ for $x \in (0,\pi)$ and $V(x) = V_0 > 0$ for $x \notin (0,\pi)$. As $V_0 \to \infty$, the number of eigenvectors for the finite well problem $-\nabla^2 + V$ also goes to infinity. Let us label by $n \in N$ the eigenvalues E_n^V in increasing order and the corresponding eigenfunctions by ϕ_n^V:

$$(-\nabla^2 + V)\phi_n^V = E_n^V \phi_n^V. \tag{11}$$

For fixed n we obtain for large values of V_0 (compare for example, Ref. 5):

$$E_n^V \simeq E_n^\infty \Big(1 - \frac{4}{\pi\sqrt{V_0}}\Big), \tag{12}$$

where $E_n^\infty = n^2$ is the infinite well energy eigenvalue with $n = 1, 2, \ldots$ We also have

$$\phi_n^V(x \leq 0) \;\simeq\; \sqrt{\frac{2}{\pi}}\left(\frac{n}{\sqrt{V_0}}\right)\exp\{-|x|\sqrt{V_0}\} \tag{13a}$$

$$\phi_n^V(0 \leq x \leq \pi) \;\simeq\; \sqrt{\frac{2}{\pi}}\Big[\sin nx + \Big(\frac{1}{\pi\sqrt{V_0}}\Big)\left[(n\pi)\cos nx - \sin nx\right]\Big] \tag{13b}$$

$$\phi_n^V(x \geq \pi) \;\simeq\; \pm\sqrt{\frac{2}{\pi}}\Big(\frac{n}{\sqrt{V_0}}\Big)\exp[-(x-\pi)\sqrt{V_0}]. \tag{13c}$$

Accordingly, when $V_0 \to \infty$, then $E_n^V \to E_n^\infty$, and

$$\phi_n^V(x) \to \phi_n^\infty(x) = \sqrt{\frac{2}{\pi}}\sin nx \tag{14}$$

for $0 \leq x \leq \pi$ and zero otherwise. The infinite well Hamiltonian eigenvalues and eigenfunctions are thus smoothly reproduced and we keep under control the accuracy of the approximation of the finite well by its infinite well idealization.

We need to achieve more than the convergence properties Eqs. (12) and (14). Namely, we are interested in verifying whether the finite well notions of position, momentum, and energy observables go through the limiting procedure. (We recall the no-go claim of Ref. 5.)

Note that the limit $\phi_n^V \rightarrow \phi_n^\infty$ as $V_0 \rightarrow \infty$ holds in the norm of $L^2(R)$. It follows that for any interval (x_1, x_2), we have, using an obvious notation, the following behavior of the localization probabilities: $P^V_{x\in(x_1,x_2)} \doteq \int_{x_1}^{x_2} |\phi_n^V(x)|^2 dx \rightarrow \int_{x_1}^{x_2} |\phi_n^\infty(x)|^2 dx = P^\infty_{x\in(x_1,x_2)}$ as $V_0 \rightarrow \infty$. So, we have secured the standard meaning of the position measurement for both the finite and infinite well problems.

These limiting behaviors are paralleled by the convergence of the suitable Fourier transforms. Indeed, it is well known that the Fourier transform, as defined in $C_0^\infty(R)$, can be extended to a unitary operator in $L^2(R)$. Therefore, the Fourier transform of ϕ_n^V also converges in the $L^2(R)$ norm to the Fourier transform $\mathcal{F}\phi_n^\infty$ of ϕ_n^∞. Hence, for any (p_1, p_2), we have that $P^V_{p\in(p_1,p_2)} \doteq \int_{p_1}^{p_2} |\mathcal{F}\phi_n^V(p)|^2 dp \rightarrow \int_{p_1}^{p_2} |\mathcal{F}\phi_n^\infty(p)|^2 dp = P^\infty_{p\in(p_1,p_2)}$ as $V_0 \rightarrow \infty$. Thus, we conclude that if the infinite well problem eigenfunctions are considered as the functions defined on R but supported by $[0, \pi]$, then we can employ the usual notions of position and momentum on R and these notions are common for the finite and the infinite well. The conceptual continuity in the notions of position, momentum, and energy measurements survives the limiting procedure $V_0 \rightarrow \infty$.

We emphasize that for $L^2(0, \pi)$, we have two nonequivalent ways of making the Fourier analysis. If $L^2(0, \pi)$ is considered as a subspace of $L^2(R)$, then $\mathcal{F}L^2(0, \pi) \subset L^2(R)$. More precisely, if $0 \neq f \in L^2(0, \pi)$, then $\mathcal{F}f \in L^2(R)$, but $\mathcal{F}f$ does not belong to $L^2(0, \pi)$. Because the support of f is compact, the function $\mathcal{F}f$ can be analytically continued to the entire complex plane. Thus, if $\mathcal{F}f$ vanishes on $R\backslash[0, \pi]$, it also vanishes identically on R.

If $R\backslash[0, \pi]$ is neglected and $L^2(0, \pi)$ is considered independently, then we can employ the Fourier series. In the language of Ref. 7, the Fourier series stands for the momentum representation formulation if the momentum operator is chosen to be P_0, as given by Eq. (2). The Hilbert space of this momentum representation is then $l^2(Z)$, the space of square summable sequences f_n, where n runs over the set of integers Z. Let us note that the self-adjoint operators, P in $L^2(R)$ and P_0 in $L^2(0, \pi)$, both exemplify the spectral theorem and the notion of momentum representation, but are fundamentally different operators.

In the course of all limiting operations, the notion of $L^2(R)$ and thus of the entire real line input (notably of the usual momentum observable) is implicit. This observation lends support to the standard momentum representation concept, employed in Refs. 3, 14, and 15, which can thus be adopted to the infinite well and the half-line wave packet dynamics. Consequently, if we had followed the strategy of Refs. 7, 5, and 8 and ignored the rest of the real line, the restriction of the model to $L^2([0,\pi])$ would have ruled out $\mathcal{F}\phi_n^\infty$. As a result, the usual concept of the momentum operator as the generator of the translation group would no longer be appropriate and the interpretation in Ref. 5 would make a sharp distinction between the finite well and infinite well cases. Such a distinction is untenable on physical grounds.

V. QUANTUM DYNAMICS WITH BARRIERS

A. Trapping as a dynamical effect

Now we shall analyze the main outcome of our previous discussion: we can make sense of various operators for trapped particles by not ignoring the rest of the real line (the exterior of the trap).

In the canonical quantization scheme, quantum mechanics on the entire real line refers to the correspondence principle, which introduces the position Q and momentum P observables as unbounded operators in $L^2(R)$. The intuitive definition of multiplication and differentiation operators on smooth functions with a reasonable fall off at infinity is sufficient to determine uniquely the conjugate self-adjoint operators that obey the canonical commutation relations in the Weyl form (that is, by means of unitary operators). This statement is purely kinematical and thus independent of any dynamics.

The free particle Hamiltonian,

$$H_f = -\frac{d^2}{dx^2} = P^2, \tag{15}$$

implies that P commutes with H_f, and thus is a constant of motion which supports the view that P is the momentum operator. For the free particle the identity (15) relates the Hamiltonian H_f and P^2. In other cases, there appear potentials or boundary conditions (such is the case for the half-line and infinite well problems). Whatever the dynamics and thus the general Hamiltonian H may be, we can safely assume that H is self-adjoint and bounded from below.

Let us consider the general mathematical mechanism of permanent confinement. Let H be a Hamiltonian operator and we choose an open interval $G \subset R$ with χ_G denoting its characteristic (indicator) function: $\chi_G(x) = 1$ for $x \in G$ and vanishes otherwise. (To conform with the previous notation, we suggest the identification $G \doteq (a,b)$ and $\overline{G} \doteq [a,b]$.)

If $f \in D(H)$, then $\chi_G f$ typically does not belong to $D(H)$. If, however, for a given H and G, the property $f \in D(H)$ necessarily implies that $\chi_G f \in D(H)$ then χ_G, considered as a projection operator in $L^2(R)$, commutes with the spectral projectors of H and hence with the unitary operator $\exp(-iHt)$. This property implies an invariance of the subspace $[f \in L^2(R); \operatorname{supp} f \subset \overline{G}]$ with respect to time evolution. Thus, if at some instant of time a particle is localized in $\overline{G}$, that is, its wave function f is supported by a subset of $\overline{G}$, then $supp\{g(t) = \exp(-iHt)f\} \subset \overline{G}$ for all times t. Hence the particle has always been in $\overline{G}$ and will stay there forever.

Consequently, if the dynamics is defined by the Hamiltonian H in $L^2(R)$, then the confinement in $\overline{G}$ occurs if and only if H can be split into a direct sum $H = H_1 \bigoplus H_2$ corresponding to the decomposition $L^2(R) = L^2(R\backslash G) \bigoplus L^2(\overline{G})$, so that H_1 is self-adjoint in $L^2(R\backslash G)$ and H_2 is self-adjoint in $L^2(\overline{G})$. Then $\exp(-iH_1t)$ and $\exp(-iH_2t)$ describe the time evolution of the system localized in $R \setminus G$ and $\overline{G}$ respectively. Moreover $\exp(-iHt) = \exp(-iH_1t)\exp(-iH_2t)$.

Thus the dynamics from the outset takes account of the impenetrable barrier at the boundary of G. This effect is purely dynamical, and there is no reason to modify the meaning of kinematical variables such as the position and momentum (see Sec. III). Consequently, if a particle described by the wave function $f(x)$ is localized in $\overline{G}$, then necessarily $f \in L^2(\overline{G})$. However, now the momentum representation reads $f(x) \to (\mathcal{F}f)(p) \doteq \tilde{f}(p)$, by the Fourier integral, Eq. (1). If G is bounded, then $\mathcal{F}f$ is an entire function. So, if a particle at some (initial) instant of time is localized in a bounded region in space, then its momentum is spread over the whole real line.

In the following we illustrate the qualitative physical and mathematical mechanisms leading to the above reduction of $L^2(R)$ by the dynamics.

B. Infinite well

First, we define $H = -\frac{d^2}{dx^2}$ through its specific domain $D(H) = [f \in AC^2(R); f, f', f'' \in L^2(R), f(0) = 0 = f(\pi)]$. We recall that the AC^2 notation refers to the absolute continuity of the first derivative which gives meaning to the second derivative (in the sense of distributions, as a measurable function). The operator $\{H, D(H)\}$ is self-adjoint and the decomposition $L^2(R) = L^2(R\backslash G) \bigoplus L^2(\overline{G})$, together with $H = H_1 \bigoplus H_2$, holds for $\overline{G} = [0, \pi]$. Thus the traditional infinite well problem is nothing else than the analysis of H_2 in the space $L^2([0,\pi])$, with the Dirichlet boundary condition. Here, $H_2 = H_w$, see for example Eq. (9).

C. Centrifugal repulsion

Let us consider the operators belonging to the family of singular problems with the centrifugal potential (possibly modified by harmonic attraction)[19,26]:

$$H = -\frac{d^2}{dx^2} + \frac{1}{[n(n-1)x^2]}, \tag{16}$$

with $n \geq 2$ and $D(H) = [f \in AC^2(R); f, f', f" \in L^2(R), f(0) = 0 = f'(0)]$. The operator H in Eq. (16) is self-adjoint. The projection operator P_+ defined by $(P_+f)(x) = \chi_{R^+}(x)f(x)$ clearly commutes with H. The singularity of the potential is sufficiently severe to enforce the boundary condition $f(0) = 0 = f'(0)$ (the generalized ground state function (cf. Ref. 25) may be chosen for this scattering problem in the form $\phi(x) = x^n$).

The Hilbert spaces $L^2(R^+)$ and $L^2(R^-)$ are invariant under the Schrödinger evolution $\exp(-iHt)$ generated by H and the Schrödinger probability current vanishes at $x = 0$ for all times. Consequently, there is no dynamically implemented communication between the two disjoint localization areas extending to the negative or positive semi-axes of R respectively. The respective localization probabilities of finding a particle on a positive or negative semi-axis are constants of the motion. Because of the singularity at 0, once trapped, a particle is confined in one particular enclosure only and cannot be detected in another.

However, we note that $D(H)$ contains functions from $L^2(R)$ that are restricted to obey $f(0) = 0 = f'(0)$ and not necessarily to vanish on either half-line. Such functions may have support on both the positive and negative semi-axes simultaneously. For example, a normalized linear combination of two components corresponding to positive and negative half-lines respectively, is a legitimate element of $D(H)$. Then, we can merely predict a probability to detect a particle on either side of the origin. This probability is a constant of the motion, and there is no probability current through the origin. In particular, due to the boundary conditions, if $f \in D(H)$ then $\chi_+ f \in D(H)$ and $\chi_- f \in D(H)$.

The classic Calogero-type problem is defined by

$$H = -\frac{d^2}{dx^2} + x^2 + \frac{\gamma}{x^2}. \tag{17}$$

The eigenvalues are $E_n = 4n+2+(1+4\gamma)^{1/2}$, where $n \geq 0$ and $\gamma > -\frac{1}{4}$, with eigenfunctions of the form:

$$f_n(x) = x^{(2\alpha+1)/2} \exp(-\frac{x^2}{2})\, L_n^\alpha(x^2) \tag{18}$$

$$L_n^\alpha(x^2) = \sum_{\nu=0}^{n} \frac{(n+\alpha)!}{(n-\nu)!(\alpha+\nu)!} \frac{(-x^2)^\nu}{\nu!}, \tag{19}$$

where $\alpha = \frac{1}{2}(1+4\gamma)^{1/2}$. The γ parameter range, $-1/4 < \gamma < 3/4$, involves some mathematical subtleties concerning the singularity at 0 that are not sufficiently severe to enforce the Dirichlet boundary condition.[22,28] However, in the range $\gamma \geq 3/4$ the ground state is doubly degenerate in the whole eigenspace of the self-adjoint operator H. The singularity at $x = 0$ decouples $(-\infty, 0)$ from $(0, +\infty)$ so that $L^2(-\infty, 0)$ and $L^2(0, +\infty)$ are the invariant subspaces for the dynamics generated by H.

The singularity in both Hamiltonians (16) and (17) can be removed by a simple replacement $x^2 \to (x^2 + \epsilon)$ with $\epsilon > 0$. The limit $\epsilon \to 0$ would restore the singularity. As with the infinite well limit for finite wells, the relatively easy to solve singular models (16) and (17) may be considered as approximations of more complicated regular (free of singularities) models.

We emphasize that impenetrable barriers are located at points where a potential singularity enforces vanishing boundary conditions. In particular, such conditions are satisfied by (generalized) ground states and this mathematical feature is responsible for the appearance of impenetrable barriers. Let $\phi \in L^2_{\text{loc}}(R)$, that is, we consider all functions that are square integrable on all compact sets in R. If there is a closed set N of Lebesgue measure zero so that (strictly speaking we admit distributions) $\frac{d\phi}{dx} \in L^2_{loc}(R \setminus N)$, then there is a uniquely determined Hamiltonian H such that ϕ is its (generalized) ground state. If $(x - x_0)^{-1/2}\phi$ is bounded in the neighborhood of x_0, then there is an impenetrable barrier at x_0. For a precise description of this mechanism in R^n, see for example, Ref. 18.

D. Multi-trapping enclosure

In contrast to the centrifugal repulsion where the singularity of the potential alone was capable of making the ground state degenerate due to the impenetrable barrier at the origin, we also can impose the existence of barriers as an external boundary condition. We introduce the differential expression $H_0 = -\frac{d^2}{dx^2}$ and observe that for any real q, the function $\psi(x) = \sin(qx)$ satisfies the equation $H_0\psi = q^2\psi$. The operator $H_q = H_0 - q^2$ is self-adjoint when operating on $D(H_q) = [f \in AC^2(R); f, f', f'' \in L^2(R), f(\frac{n\pi}{q}) = 0, n = 0, \pm1, \pm2, \ldots]$ and $\sin(qx)$ is its generalized ground state. In this case a particle localized at time 0 in a segment $[(n-1)\frac{\pi}{q}, n\frac{\pi}{q}]$ will be confined there forever. This model can be considered as that of multi-trapping enclosures, with impenetrable barriers at points $n\frac{\pi}{q}$. Note that in every segment $[(n-1)\frac{\pi}{q}, n\frac{\pi}{q}]$, the corresponding dynamics is identical with the one associated previously with the infinite well.

VI. CONCLUSION

We have considered several singular models (such as the infinite well) that serve as approximations of regular ones (such as the finite well) in the sense of suitable limits. If the properties of the limiting model are to give a reliable, albeit approximate, description of a non-singular one, the physical meaning of the observables should survive the limiting procedure. As we have demonstrated, such a viewpoint is consistent with localized dynamics in the presence of traps modelled by impenetrable barriers.

There is one common feature shared by the models considered in Secs. III–V: the Hamiltonian is a well defined self-adjoint operator in each case, respecting various confinement requirements by suitable boundary conditions. There is however no consistent canonical quantization procedure that can be carried out exclusively in the trap interior, because in the case of Dirichlet boundary conditions there is no self-adjoint momentum-like operator. If we do not ignore the exterior of the trap the momentum observable paradoxes disappear and the canonical quantization procedure reduces to its textbook meaning also in the presence of impenetrable barriers.

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APPENDIX A: BASIC MATHEMATICAL CONCEPTS

We shall give a brief introduction to the basic mathematical concepts employed in the paper, with an emphasis on the distinctions between symmetric and self-adjoint operators in Hilbert space.

(1) *Absolute continuity.* Let $\phi(x)$ be locally integrable on R. Then $f(x) = \int_a^x \phi(t)dt$ is called absolutely continuous and denoted by $f \in AC(R)$. If ϕ is continuous, then f is differentiable and $\frac{df(x)}{dx} = \phi(x)$. If $\frac{d}{dx}$ is understood as an operator in Hilbert space and its domain contains absolutely continuous functions, then we set $\frac{df(x)}{dx} = \phi(x)$, even if f happens not to be differentiable.

(2) *Domains of operators.* Most of the operators discussed in this paper are unbounded. When defining an unbounded operator, it always is necessary to specify its domain of definition. If A is an operator in the Hilbert space $\mathcal{H}$, we write $D(A) \subset \mathcal{H}$ for the domain of A. An operator B is called an extension of A, which is often written as $A \subset B$, if and only if $D(A) \subset D(B)$ and $Af = Bf$ for all $f \in D(A)$.

(3) *Symmetric versus self-adjoint operators.* An operator B is adjoint to A if (a) $(g, Af) = (Bg, f)$ for all $f \in D(A)$ and $g \in D(B)$, (b) B is a maximal operator with the property (a), in the sense that if $B \subset C$ and $B \neq C$, then (a) does not hold for C. We write $B = A^*$ if B is adjoint to A. It follows that $A \subset C$ implies $C^* \subset A^*$. We say that A is symmetric if $A \subset A^*$ and self-adjoint if $A = A^*$.

(4) *Closed operator.* Let us consider a densely defined operator A. For any $g \in D(A)$, we set $||g||_1 = [(Ag, Ag) + (g, g)]^{1/2}$. Then $|| \cdot ||_1$ is a norm in $D(A)$. If $f_n \in D(A)$ is a Cauchy sequence in $|| \cdot ||_1$, that is, $\lim_{n,m\to\infty} ||f_m - f_n||_1 = 0$, then f_n also is a Cauchy sequence in the Hilbert space $\mathcal{H}$ norm $||f|| = [(f, f)]^{1/2}$. By the completeness of $\mathcal{H}$ there is $f \in \mathcal{H}$ such that $\lim_{n\to\infty} ||f - f_n|| = 0$. If it follows that f necessarily belongs to $D(A)$ (that is, $D(A)$ is complete in the $|| \cdot ||_1$ norm), then we say that A is closed and we write $A = \overline{A}$. If A is not closed, it still may have a closed extension. That can be guaranteed by assuming $D(A^*)$ to be dense in $\mathcal{H}$.

Under such circumstances the $||\cdot||_1$-norm limit $\lim_{n\to\infty} Af_n$ exists for any Cauchy sequence $f_n \in D(A)$ and moreover $g = \lim_{n\to\infty} Af_n$ is the same for all sequences f_n converging to the same limit f. Thus we may define $\overline{A}f = \lim_{n\to\infty} Af_n$. The operator $\overline{A}$ is a minimal closed extension of A; $\overline{A}$ is called a closure of A. We have $A^* = (\overline{A})^*$, $\overline{A^*} = A^*$.

(5) *Self-adjoint extension.* Let A be symmetric, $A \subset A^*$ but is not necessarily self-adjoint. The closure $\overline{A}$ of A obeys $A \subset \overline{A} \subset A^*$. Even if $A \neq A^*$, we may have $\overline{A} = A^*$ and then A is called essentially self-adjoint. However, typically we may expect that $A^* \neq \overline{A}$ and at this point we need to invoke the notion of the self-adjoint extension.

Suppose that B is a symmetric extension of $\overline{A}$, then $\overline{A} \subset B \subset B^* \subset A^*$. Can we extend $\overline{A}$ so that $\overline{A} \subset B = B^* \subset A^*$, that is, has $\overline{A}$ a self-adjoint extension? If so, is this extension unique? The full answer to those questions is given by the Krein-von Neumannn theory of self-adjoint extensions of symmetric operators[23] which we shall invoke in the following.

(6) *Deficiency indices and self-adjoint extensions.* Let A be a closed operator, that is, $A = \overline{A}$. We denote by $\mathcal{M}, \mathcal{N} \subset \mathcal{H}$ the spaces of the solutions of $(A^* \mp i)g = 0$ and by m and n respective dimensions of these spaces. The numbers n, m are called deficiency indices for A. For simplicity, we assume m and n to be finite. Then, A has self-adjoint extensions if and only if $n = m$. Let the deficiency indices of A form a pair (n, n). Then there is a one-to-one correspondence between the self-adjoint extensions of A and the family of all unitary $n \times n$ matrices. We consider some examples in the following.

(a) Consider $\mathcal{H} = L^2(a, b)$ and $A = -i\frac{d}{dx}$ acting in $D(A) = C_0^\infty(a, b) \subset L^2(a, b)$. We recall that $f \in C_0^\infty(a, b)$ if and only if f is infinitely differentiable and $\operatorname{supp} f \subset (a, b)$. Accordingly, $\overline{A} = -i\frac{d}{dx}$ with the domain $D(\overline{A}) = \{f \in AC(a, b); f(a) = f(b) = 0\}$. Integration by parts shows that $A^* = \overline{A}^* = -i\frac{d}{dx}$ with $D(A^*) = AC(a, b)$. Thus $\overline{A} \subset A^*$, that is, $\overline{A}$ is a closed symmetric operator and the equations $(A^* \mp i)g = 0$ take the form $(-i\frac{d}{dx} \mp i)g = 0$. The solutions are $\exp(\mp x)$, and hence $m = \dim \mathcal{M} = \dim \mathcal{N} = 1$, and the family of self-adjoint extensions is indexed by $\exp(i\alpha)$ with $0 \leq \alpha < 2\pi$. The self-adjoint extensions are determined in terms of the boundary conditions; $A_\alpha = A_\alpha^* = -i\frac{d}{dx}$ with respective domains $D(A_\alpha) = \{f \in AC(a, b);\ f(a) = \exp(i\alpha)f(b)\}$.

(b) Consider $H = -\frac{d^2}{dx^2}$ with $D(H) = C_0^\infty(a, b)$. Then we have $\overline{H} = -\frac{d^2}{dx^2}$ with the domain $D(\overline{H}) = \{f \in AC^2(a, b);\ f(a) = f(b) = f'(a) = f'(b) = 0\}$, where $AC^2(a, b)$ denotes functions with absolutely continuous first derivatives. Two integrations by parts show that $\overline{H}$ is symmetric and $H^* = -\frac{d^2}{dx^2}$ acts in the domain $D(H^*) = AC^2(a, b)$. The deficiency indices of H^* follow from $(-\frac{d^2}{dx^2} \mp i)g = 0$. In both cases we obtain the same pair of linearly independent solutions: $\exp(\pm kx)$ with $k = (1 - \sqrt{2})(1 + i)/\sqrt{2}$. Therefore, $\mathcal{M} = \mathcal{N}$ and $m = n = 2$.

(c) Now let $a = 0$ and $b = \infty$, that is, $\mathcal{H} = L^2(0, \infty)$. In this case, $\exp(x)$ is not an element of $\mathcal{H}$, and $\exp(-x) \in \mathcal{H}$. Thus $m = 0$ and $n = 1$, and hence there is no self-adjoint extension of $A = -i\frac{d}{dx}$. On the other hand, the same reasoning for $\overline{H}$ implies that $m = n = 1$, and thus there is a one-parameter family of self-adjoint extensions on the half-line.

(d) If we choose $a = -\infty$ and $b = +\infty$, that is, $\mathcal{H} = L^2(R)$, we have $m = n = 0$ for both $\overline{A}$ and $\overline{H}$. Therefore in this case, both A and H are essentially self-adjoint.

(7) *Spectral theorem.* The spectral theorem describes self-adjoint operators in terms of projection operators. We shall describe how it works for operators discussed in the paper.

For each $0 \leq \alpha < 2\pi$ the family $\{e_n^\alpha(x); n = 0, \pm 1, \pm 2, \ldots\}$ defined by Eq. (3) is an orthonormal basis in $L^2([0,\pi])$. We denote by Q_n^α the projection operator onto the one dimensional space spanned by the $e_n^\alpha(x)$. The operator P_α, Eq. (2), can be written as $P_\alpha = \sum_{n=-\infty}^{n=+\infty}(2n + \frac{\alpha}{\pi})Q_n^\alpha$. The condition for f to be in the domain $D(P_\alpha)$ of P_α follows by direct calculation, see for example, our comment below Eq. (4). Now, we can define functions of P_α, for example $H_\alpha = P_\alpha^2 = \sum_{-\infty}^{+\infty}(2n + \frac{\alpha}{\pi})^2 Q_n^\alpha$ with $D(P_\alpha^2)$ given by Eq. (7). Similarly $\exp(-iH_\alpha t) = \sum_{-\infty}^{+\infty} \exp[-i(2n + \frac{\alpha}{\pi})^2 t]\, Q_n^\alpha$. Note that although both P_α and P_α^2 are unbounded, the operator $\exp(-iP_\alpha^2 t)$ is bounded and defined on the whole of $L^2([0,\pi])$.

(8) *Momentum representation.* We introduce the notion $\tilde{P}$ of the "momentum operator in the momentum representation": $\tilde{P}f(p) = pf(p)$; $D(\tilde{P}) = \{f \in L^2(R); \int |pf(p)|^2 dp < \infty\}$. We also have $\tilde{P}^2 f(p) = p^2 f(p)$; $D(\tilde{P}^2) = \{f \in L^2(R); \int |p^2 f(p)|^2 dp < \infty\}$. The operator $\exp(-i\tilde{P}^2 t)f(p) = \exp(-ip^2 t)f(p)$ is bounded and defined on the whole of $L^2(R)$.

If $\mathcal{F}$ stands for the Fourier transformation and $\mathcal{F}^{-1}$ for its inverse, then $P = \mathcal{F}^{-1}\tilde{P}\mathcal{F}$ and $D(P) = \mathcal{F}^{-1}D(\tilde{P})$. Analogously we have $P^2 = \mathcal{F}^{-1}\tilde{P}^2\mathcal{F}$; $D(P^2) = \mathcal{F}^{-1}D(\tilde{P}^2)$ and $\exp(-iP^2 t) = \mathcal{F}^{-1}\exp(-i\tilde{P}^2 t)\mathcal{F}$.

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