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THE QUANTUM OSCILLATOR IN PHASE SPACE
Part I

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Starting with a real abstract algebra which encapsulates the algebraic structures of both classical and quantum mechanics, this paper presents a self–contained realization of the latter in phase space. Having both mechanics formulated in the same space opens two new windows into the comparative study of foundations. This stems from the fact that the same physical problem, as defined by a given Hamiltonian, can be solved in several independent ways. The exact solutions can then be compared. Thus, comparison of the classical and quantum solutions in phase space offers new epistemological insights into Bohr's correspondence principle, while comparison of the quantum solutions in the different formalisms of Hilbert space and phase space yields new physical insights. These general ideas are then tested on the harmonic oscillator. The analytic ground work is presented in Part I, the exact solutions will be derived in Part II.

1. *Introduction*

A pre–geometric algebraic structure, referred to as "quantal algebra," has been introduced in 1976 by A. Petersen and one of us [1] to encapsulate the common characteristics of classical and quantum mechanics and to exhibit as clearly as possible Bohr's correspondence principle. A theory is "pre-geometric" if it neither requires, nor makes reference to, the geometric structure of space.

Realizations of this quantal algebra include not only classical and quantum mechanics in their standard canonical and Heisenberg formulations, but also a new realization in phase space, which is quantum mechanical in structure but very similar to classical mechanics in formulation. We refer to this formulation as *phase space quantum mechanics.* In this realization, observables and states are real C^∞ functions over phase space, just as in classical mechanics, but their multiplicative and Lie structures obey the identities that characterize quantum mechanics. The fact that the states are functions over phase space ($2n$ dimensions) rather than over position space (n dimensions) makes this theory appear formally richer than Hilbert space quantum mechanics. Only careful analysis will show if the apparent difference is physically interesting. The first impression might be that the Heisenberg uncertainty relations are violated, but, as the solution of the harmonic oscillator indicates, this is probably not the case. The reason is that the real phase space functions which represent states are not everywhere non-negative, even though their integral over the entire phase space equals one. Consequently, they are not ordinary probability densities. Like Schwartz distributions (e.g., the Dirac delta function), these states acquire observable meaning only after integration — but they differ from distributions in at least three essential points: (a) while the distributions are not true functions (i.e., are not defined as point-to-point maps), our states are everywhere of class C^∞, or even analytic, as in the case of the harmonic oscillator, (b) unlike distributions, they "act" non-locally in the sense that their algebraic products involve derivatives to infinite order, and (c) unlike distributions, they may not be integrated over domains of arbitrarily small measure. This last point requires clarification: even though the computation of the expectation values of observables is the same as in classical mechanics, the domains of integration cannot be simultaneously arbitrarily small and located anywhere in phase space. If the domain of integration is allowed to be arbitrarily small, positive definite observables can have negative expectation values and, as a corollary, probabilities are not confined to the interval $[0, 1]$.

In the present work, we study the time-independent harmonic oscillator. We first solve the problem in the self-contained formalism of phase space quantum mechanics, and then we compare the results with the standard quantum mechanical solution. Although the thinking and formalism are very different from what we are accustomed to in Hilbert space quantum mechanics, the observable results — stationary energy levels and probability distributions in position space — are exactly the same. Moreover, since the classical solutions are defined in the same phase space, we can compare the quantum and classical solutions at levels of detail not accessible in other formalisms.

Historically, the Lie structure of phase space quantum mechanics, which is a transcendental generalization of the Poisson bracket, was known long before it was algebraically derived in Ref. 1 — see Refs. 2 and 3. It has been referred to as the "Moyal bracket", or "sine bracket". We call it the "Lie product", or, suggesting its anti-symmetry, the "α -product". In addition to the Lie product, the quantal algebra has an additional structure, which we call the "Jordan product", or, suggesting its symmetry, the "σ-product". While it is true that the Lie and Jordan products are not mutually independent (since exactly two pairs of such products exist, as shown in Ref. 1, it is evident that, given one product, the other one is uniquely determined), both must be explicitly defined for quantum mechanics in phase space to be self-contained. Indeed, they play complementary roles. The σ-product is the source of spectra (eigenvalues and eigenstates), while the α-product is at the foundations of dynamics. The present work contains the complete investigation of the σ-product in the case of the simplest but very important bound system, the stationary harmonic oscillator. We use the α-product only to impose time–independence.

For phase space quantum mechanics to be equivalent to the standard Hilbert space theory, both formalisms must yield the same probabilities whenever comparison is possible. In Hilbert space, the states are complex functions, $\psi(x)$, which, according to Born, acquire the physical meaning of probability density in x by way of the modulus squared, i.e., $\rho_h(x) = \psi(x)\bar{\psi}(x)$. In phase space, the states are real (both positive and negative) functions, $u(x,p)$, which, by analogy with classical mechanics — but for the mentioned exception related to the size of the integration domain — acquire the physical meaning of probability density in x by integration, i.e., $\rho_p(x) = \int\limits_{-\infty}^{\infty} u(x,p)\mathrm{d}p$. For the harmonic oscillator, we shall prove that $\rho_h(x) = \rho_p(x)$.

2. *Overview of abstract mechanics*

The theoretical basis for the present work is the purely algebraic Grgin-Petersen article mentioned above. Our objective at the time was to take seriously Bohr's belief, as he had often expressed it orally to Petersen, that there should be more to the correspondence principle than was then understood. It seems evident that what limits the understanding of the relationship between classical and quantum mechanics is the dissimilarity of the formalisms in which these theories are couched. Indeed, the languages of phase space and of Hilbert space are worlds apart. Consequently, the perceived differences between classical and quantum mechanics are partly due to differences in the supporting formalism — differences which may not be fundamental by themselves but mask the essential ones. To pursue Bohr's intuition, we sought a formulation of mechanics that would be common to both theories, a formulation that would maximally exhibit the common structures of these theories, while concentrating the differences in, ideally, a single place. These heuristics led us to an abstract algebra of observables among whose realizations is a unique phase space formulation of quantum mechanics. Justifying them as much as possible intuitively, we shall now concisely review the concepts of this abstract mechanics. Except for the proofs, which are given in Ref. 1, the following review is complete, making this paper self–contained.

In addition to observables, we shall also need states and expectation values

— concepts we had not investigated in Ref. 1. Borrowing the fact from standard quantum mechanics, we here define the states as *idempotent observables.*

2.1. The algebraic structure of observables

2.1.1. The linear space of observables

We use the terms "dynamical variable" and "observable" interchangeably. In classical mechanics, observables are represented by real C^∞ functions over a phase space; in quantum mechanics, by Hermitian operators in a Hilbert space. In both cases they form a real linear space. Hence, to arrive at a structure common to both mechanics, we first introduce a real linear space, $\mathcal{H}$, whose points we call *abstract observables* . We denote these observables by small Roman letters, $f, g, h... \in \mathcal{H}$.

2.1.2. The Jordan product

In classical mechanics, the dynamical variables can be multiplied by each other to produce new observables (products of C^∞ functions are C^∞ functions). Hence, the classical observables form an associative and commutative algebra (usually referred to as the ring of continuous functions). In quantum mechanics, there are two possibilities. To form new operators, one can use either the associative product, or the symmetric product. The computational advantage of the former is associativity, but it does not preserve the space of observables. This is due to the fact that the associative product of two arbitrary Hermitian operators is not Hermitian. By contrast, the non associative symmetric product of two Hermitian operators, A, B, defined as

$$\{A, B\} = \frac{1}{2}(AB + BA), \tag{1}$$

is Hermitian, and hence plays the same structural role as the product of functions in classical mechanics. Which of the two operator products should be taken as the basis for quantum mechanics is a matter of viewpoint concerning foundations. Let us consider both possibilities in turn.

If it is taken as axiomatic that observables must be represented by operators, then the associative product is the natural one. This is the attitude that has prevailed since the early days of quantum theory. The well–known algebraic re–formulations of quantum mechanics, like the various star–algebras, assume associativity.

On the other hand, if it is the real structure of observables that is taken to be fundamental, all relevant operations must preserve it. Since the associative product is not structure-preserving in quantum theory, and since nothing fundamental would favour associativity in an abstract algebra initially free of interpretation, it is the symmetric product (1) that imposes itself in this abstract approach. It is interesting to note that the algebraic viewpoint that preserves the reality of observables had been favoured by Pascual Jordan in the early days of modern quantum theory [4,5], so that the product (1) bears his name. This approach lost its appeal, however, when it was shown not to be more general than the Von Neuman formalism [6]. As a consequence, it has not been developed far enough to reach the problem–solving stage. To the best of our knowledge, the present work is the first that offers the exact analytic solution of a physical problem in a real algebra based on the Jordan product. This solution is obtained *strictly within the real theory* — not translated into it from the known Hilbert space solution.

To represent abstractly the real products of both classical and quantum mechanics, we introduce into the linear space $\mathcal{H}$ a symmetric, but not necessarily associative, product, which we denote by σ:

$$f\sigma g = g\sigma f \tag{2}$$

This promotes the linear space $\mathcal{H}$ into an algebra. Since both classical and quantum mechanics have a unit observable (the real constant 1 and the unit operator I, respectively), we equip the algebra $\mathcal{H}$ with a unit, denoted by $e \in \mathcal{H}$. Thus $e\,\sigma f = f$ for all $f \in \mathcal{H}$.

In classical mechanics, the product σ is associative; in quantum mechanics it is not. The lack of associativity in an algebra is "measured" by the *associator*, a linear mapping, $[\,,\,,] : \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \longrightarrow \mathcal{H}$, defined by the relation

$$[f, g, h] = (f\sigma g)\,\sigma h - f\sigma\,(g\sigma h)\,. \tag{3}$$

Just as the commutator is a key concept in standard quantum mechanics, the associator is a key concept in our abstract mechanics. Obviously, $[f, g, h] = 0$ in the classical theory.

2.1.3. The Lie product

Given an algebra, $\{\mathcal{H}, \sigma\}$ in our case, one also considers its Lie group of automorphisms, i.e., the group of linear mappings, A, of the space $\mathcal{H}$ onto itself which preserve the product:

$$A(f\sigma g) = (Af)\sigma(Ag).$$

Infinitesimally, these transformations are generated by derivations:

$$D\,(f\sigma g) = (Df)\,\sigma g + f\sigma\,(Dg)\,,$$

where $A = I + \varepsilon D$. The totality of all derivation operators D is a Lie algebra. The Lie product in this algebra is the commutator. In both classical and quantum mechanics these derivations are of the "inner" type, which means that a derivation operator is associated with every observable, and that there are no other derivation operators.

In classical mechanics, a derivation operator is associated to an observable *via* the Poisson bracket. If x and p are the position and momentum coordinates in a 2-dimensional phase space, and if $g = g(x,p)$ is an arbitrary observable, the derivation operator D_g is

$$D_g = \{g, \} = \frac{\partial g}{\partial p}\frac{\partial}{\partial x} - \frac{\partial g}{\partial x}\frac{\partial}{\partial p}. \tag{4}$$

In quantum mechanics, a derivation operator is associated to an observable *via* the commutator. Thus, if g is a Hermitian operator,

$$D_g = \tfrac{1}{i}\,[g,\ ]\,.$$

When an observable, as g in these examples, is used to define a derivation, it is referred to as a *generator* (it generates an infinitesimal transformation). *It is characteristic of mechanics, both classical and quantum, that observables and generators coincide*, a fact strongly emphasized by Dirac.

It follows from these remarks that the abstract algebra $\{\mathcal{H}, \sigma\}$ must also be equipped with a Lie product — the abstract counterpart of the Poisson bracket and of the commutator. We denote this product by α. In addition to the symmetry relation (2), the following identities then hold in the two-product algebraic structure $\{\mathcal{H}, \sigma, \alpha\}$:

Antisymmetry of α:

$$f\alpha g + g\alpha f = 0. \tag{5}$$

Jacobi identity for α:

$$(f\alpha g)\,\alpha h + (h\alpha f)\,\alpha g + (g\alpha h)\,\alpha f = 0. \tag{6}$$

Derivation of α with respect to σ:

$$f\alpha\,(g\sigma h) = (f\alpha g)\,\sigma h + g\sigma\,(f\alpha h)\,. \tag{7}$$

In order to complete this set of defining identities for $\{\mathcal{H}, \sigma, \alpha\}$, we need to discover an additional one that would restrict the still arbitrary associator, Eq. (3). To this end, we introduce a new product, β, which is to be the abstract counterpart of the associative product of operators in Hilbert space. Hence, β is defined as

$$\beta = \sigma + ib\alpha. \tag{8}$$

This short-hand notation represents the identity $f\beta g = f\sigma g + ibf\alpha g$ for some real number b. Obviously, $\mathcal{H}$ is not closed under β, but its complexification $\mathcal{H} \oplus \mathrm{i}\,\mathcal{H}$ is. We require associativity to hold in the complex algebra, i.e.,

$$(f\beta g)\,\beta h = f\beta\,(g\beta h)\,. \tag{9}$$

By substituting for β its definition (8) and working out the algebra using the Jacobi and derivation identities, Eqs. (6) and (7), one obtains a new identity

$$[f, g, h] = ag\alpha\,(h\alpha f)\,, \tag{10}$$

where $a = b^2$ is a non-negative real number. Even though this relation is derived by complexification of the underlying linear space, we assume it to be defining for the real quantal algebra $\{\mathcal{H}, \sigma, \alpha\}$. We note, however, that the present approach is only a short-cut, heuristically sufficient for the present overview of quantal algebra. A proof that remains within the field of real numbers and does not rely on the associativity of operators in Hilbert space is given in Ref. 1.

This completes the review of the abstract algebraic structure of mechanics. The distinction between the classical and quantum versions is localized at one place only, in the association relation (10). The two theories are characterized, respectively, by $a = 0$ and $a > 0$. In the latter case, a can be normalized to unity by re-scaling α (specifically, by the transformation $\alpha \to \alpha/b$). Obviously, the existence of the unit, $e\sigma e = e$, fixes the scale of σ. Re-scaling α, we get the final form

$$[f, g, h] = g\alpha\,(h\alpha f) \tag{11}$$

for the quantum mechanical association identity.

2.1.4. The states

Borrowing from standard quantum mechanics the fact that the states are Hermitian idempotents (in Dirac's notation, if $<\,|\,>= 1$ and $u = |\,><\,|$, then $uu = u$), we propose the following definition of abstract states:

Definition 2.1 *The pure abstract states are the observables $u \in \mathcal{H}$ which satisfy the idempotence condition*

$$u\sigma u = u. \tag{12}$$

2.1.5. The expectation values

In quantum mechanics, the expectation value of an observable f in a state $u = |\,><\,|$ is

$$\langle f\rangle_u = \langle\,|f|\,\rangle = \mathrm{Tr}(f|\,><\,|) = \mathrm{Tr}\,(fu)\,.$$

In order to take over this relation as the tentative definition of expectation values in abstract mechanics, we assume the existence of an appropriate linear functional, denoted by T, which is to correspond to the trace.

Definition 2.2 *The expectation value of an observable f in a state u is*

$$\langle f\rangle_u = \mathrm{T}\,(f\sigma u)\,. \tag{13}$$

The self–evident requirement that the expectation value of a constant, λ, (stated more accurately, of a constant observable, λe) should be that same constant, i.e., $\langle \lambda e \rangle_u = \lambda$, implies the norm condition

$$\mathrm{T}\,(e\sigma u) \equiv \mathrm{T}\,(u) = 1 \tag{14}$$

on the states.

2.1.6. *Eigenvalues and eigenvectors*

If u_λ satisfies the characteristic equation

$$f\sigma u_\lambda = \lambda u_\lambda \tag{15}$$

for some $\lambda \in \mathcal{R}$, then, by relations (13) and (14),

$$\langle f \rangle_{u_\lambda} = \lambda, \tag{16}$$

i.e., the expectation value of an observable in one of its eigen-state is the corresponding eigen-value.

The algorithmic definition of T is realization-dependent. It is the trace of a matrix in standard quantum mechanics, the integral over phase space in classical mechanics. It is this latter realization that carries over to quantum mechanics in phase space. Hence, we use the definition

$$\mathrm{T}f = \int\limits_{\Phi} f(x,p)\mathrm{d}x\mathrm{d}p. \tag{17}$$

Combining (14) and (17), we get the normalization condition for the states

$$\int\limits_{\Phi} u(x,p)\mathrm{d}x\mathrm{d}p = 1. \tag{18}$$

2.1.7. *Orthogonality*

The orthogonality of states that belong to non-degenerate eigenvalues is usually presented as a Hilbert space theorem, but it can be derived abstractly. This makes it valid in any realization of quantum mechanics.

Definition 2.3 *Two observables, f, g, are said to be* sigma orthogonal *if their σ product vanishes: $f\sigma g = 0$.*

Theorem 2.1 The sigma orthogonality theorem. *If the eigenvalues of an observable, f, are not degenerate, and if its eigenvectors, u_λ, are constants of the motion with respect to f, i.e., if $f\alpha u_\lambda = 0$, then the eigenvectors are idempotent and mutually sigma-orthogonal.*

Proof. Let λ and μ be eigen-values of f:

$$\begin{aligned} f\sigma u_\lambda &= \lambda u_\lambda, \\ f\sigma u_\mu &= \mu u_\mu. \end{aligned}$$

Consider the associator $[f, u_\lambda, u_\mu]$. From the association and derivation identities (3) and (11) follows

$$(f\sigma u_\lambda)\,\sigma u_\mu - f\sigma\,(u_\lambda \sigma u_\mu) = u_\lambda \alpha\,(u_\mu \alpha f)\,.$$

By the assumption of the theorem, the right-hand side vanishes. Hence

$$f\sigma\,(u_\lambda \sigma u_\mu) = \lambda\,(u_\lambda \sigma u_\mu)\,.$$

Since σ is symmetric, interchanging λ and μ yields

$$f\sigma\,(u_\lambda \sigma u_\mu) = \mu\,(u_\lambda \sigma u_\mu)\,.$$

The difference of these two equations is

$$(\lambda - \mu)\,(u_\lambda \sigma u_\mu) = 0.$$

Hence, for $\lambda \neq \mu$ the states u_λ, u_μ are sigma-orthogonal. For $\lambda = \mu$ we get

$$f\sigma\,(u_\lambda \sigma u_\lambda) = \lambda\,(u_\lambda \sigma u_\lambda)\,.$$

Since, by assumption, λ is not degenerate, $(u_\lambda \sigma u_\lambda)$ is unique up to a constant coefficient. By relation (15), it must then be proportional to u_λ. Hence:

$$u_\lambda \sigma u_\mu = A u_\lambda \delta_{\lambda\mu}. \tag{19}$$

3. *The harmonic oscillator*

Using mass and angular frequency as parameters, the harmonic oscillator is defined in phase space by the Hamiltonian

$$H = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2. \tag{20}$$

For some energy, E, the classical phase space orbit is given by the functions

$$x = \sqrt{2E/m\omega^2}\,\sin(\omega t)\,, \tag{21}$$

$$p = \sqrt{2Em}\,\cos(\omega t)\,. \tag{22}$$

These equations are our starting point for the development of the corresponding quantal formalism in phase space. The Hamiltonian is the same in both theories, while the orbit, an asymptotic concept in Hilbert space quantum mechanics, is in phase space a boundary between the oscillating and non-oscillating behaviours of quantum states.

3.1. A dimensionless formalism

Since the quantal formalism in phase space is based on transcendental, hence inhomogeneous, functions of the dynamical variables, the theory must be formulated in terms of dimensionless variables. We thus replace the four physical variables p, x, t and H,by dimensionless ones, $\eta, \xi, \tau \in \mathcal{R}$, and $\chi \in \mathcal{R}^+$, according to the relations

$$\begin{aligned} p &= P_0\eta, && (23)\\ x &= L_0\xi, && (24)\\ H &= E_0\chi, && (25)\\ t &= T_0\tau. && (26) \end{aligned}$$

The coefficients P_0 to T_0 are constants of appropriate dimensions. To construct them, one needs three dimensionally independent constants. Two are provided by the Hamiltonian itself: the mass m, and the angular frequency ω; the third is Planck's quantum of action, h. We shall use $\hbar$, which is often equated to one. Except for arbitrary dimensionless coefficients, which we may take to be equal to one throughout, dimensional analysis yields the solutions

$$\begin{aligned} P_0 &= \sqrt{\hbar\omega m}, && (27)\\ L_0 &= \sqrt{\hbar/\omega m}, && (28)\\ E_0 &= \hbar\omega, && (29)\\ T_0 &= 2\pi/\omega. && (30) \end{aligned}$$

We shall write the energy of the oscillator in terms of the energy constant E_0 and of a dimensionless coefficient λ:

$$E = \lambda E_0. \qquad (31)$$

The orbit, Eqs. (21) and (22), is then a circle in phase space:

$$\begin{aligned} \xi &= \sqrt{2\lambda}\sin\tau, && (32)\\ \eta &= \sqrt{2\lambda}\cos\tau. && (33) \end{aligned}$$

For the dimensionless Hamiltonian χ, one obtains

$$\chi = H/E_0 = \frac{1}{2}\left(\xi^2 + \eta^2\right). \qquad (34)$$

One more phase space structure, integration, is to be expressed in dimensionless coordinates. In physical coordinates, the differential measure is simply $\mathrm{d}p\mathrm{d}x$, as in formula (17). In dimensionless coordinates, it is not necessarily $d\xi d\eta$, but it is proportional to it. Hence, we define the trace as

$$\mathrm{T}f = N \int_{\Phi} f(\xi,\eta) d\xi d\eta. \tag{35}$$

The normalization constant N remains to be determined. It contains two components: the Jacobian of the transformations (23) (24), which is $P_0 L_0 = \hbar = 1$, and a contribution from a parameter, c, which will be introduced in the next section. Hence, the value of N will be selected later.

This completes the transition to dimensionless variables. We next review in these coordinates the classical and quantum mechanical concepts we shall be referring to later.

3.2. Classical dynamics

In the phase space Φ of canonical variables ξ, η, the algebra of dynamical variables is the class of C^∞ functions. The Poisson bracket

$$\{f,g\} = \frac{\partial f}{\partial \eta}\frac{\partial g}{\partial \xi} - \frac{\partial f}{\partial \xi}\frac{\partial g}{\partial \eta} \tag{36}$$

defines dynamics. While this symbol is typographically adequate for classical mechanics, it is very inconvenient for the analytic development of quantum mechanics in phase space, where one has to take all the powers of the operation it represents. To remedy this difficulty, we shall use the following product-like symbol to represent the bilinear map defined by relation (36):

$$\overset{\leftrightarrow}{\nabla} = \overset{\leftarrow}{\partial_\eta}\overset{\rightarrow}{\partial_\xi} - \overset{\leftarrow}{\partial_\xi}\overset{\rightarrow}{\partial_\eta}. \tag{37}$$

The bidirectional arrow indicates that one derivative acts to the left and one to the right. We shall drop it for simplicity, as there will be no occasion for confusion with the gradient operator of vector analysis. Thus, we write $f\nabla g \equiv \{f,g\}$. We shall refer to the symbol "∇" as "the Poisson product". Clearly, it is the Lie product of a quantal algebra, i.e., it satisfies the identities (5), (6) and (7) if one takes $\alpha = \nabla$, and if one takes for σ the ordinary product of functions.

In general, for any dynamical variable f, the expression $f\nabla$ represents a differential linear operator in the space of dynamical variables. In particular, the Hamiltonian (34) generates the rotation operator in the phase space Φ:

$$\chi\nabla = \eta\partial_\xi - \xi\partial_\eta. \tag{38}$$

Like the concept of "circle", the concept of "rotation" is not structural in phase space, where there is no Euclidean metric. It is nevertheless a convenient concept as long as one remains within the same coordinate system — as we do in the present work.

3.3. Classical expectation values

The other concepts of classical mechanics whose quantum mechanical counterparts we are interested in are integration over phase space and expectation values. General states are distributions in Φ, i.e., non-negative functions, $\rho(\xi,\eta)$, whose integral over phase space is equal to one:

$$\rho(\xi,\eta) \geq 0, \tag{39}$$

$$\int\limits_{\Phi} \rho(\xi,\eta)\, \mathrm{d}\xi \mathrm{d}\eta = 1. \tag{40}$$

For any dynamical variable, f, the expectation value in the state ρ is then given by the integral

$$\langle f \rangle_\rho = \int\limits_{\Phi} f(\xi,\eta)\, \rho(\xi,\eta)\, \mathrm{d}\xi \mathrm{d}\eta. \tag{41}$$

The pure states are delta functions,

$$\rho(\xi,\eta) = \delta(\xi - \xi_0)\, \delta(\eta - \eta_0),$$

whose anchor points $(\xi_0,\ \eta_0)$ are functions of time and move along classical phase space orbits.

3.4. The quantum mechanical oscillator

In dimensionless variables, the Schrödinger quantization procedure $x \to x$, $p \to -i\hbar\partial_x$, reads:

$$\begin{aligned} \xi &\to \xi, \\ \eta &\to -i\partial_\xi, \end{aligned}$$

and the Hamiltonian (34) is an operator in Hilbert space:

$$\widehat{\chi} = \frac{1}{2}\left(\xi^2 - \partial_\xi^2\right). \tag{42}$$

The time-independent Schrödinger equation

$$\widehat{\chi}\psi = \lambda\psi$$

has the well-known solutions

$$\psi_n(\xi) = A_n H_n(\xi)\, e^{-\xi^2/2}, \tag{43}$$

$$\lambda = n + \frac{1}{2}, \tag{44}$$

$$A_n = \left[\sqrt{\pi} 2^n n!\right]^{-1/2}. \tag{45}$$

The probability density function $\rho(\xi) = |\psi(\xi)|^2$ is then

$$\rho_n(\xi) = \frac{1}{\sqrt{\pi} 2^n n!} H_n^2(\xi)\, e^{-\xi^2}. \tag{46}$$

These standard formulae are listed here in dimensionless coordinates for future reference. The following step is non-standard. It is needed here for comparison with our later results.

We shall need the probability distribution $\rho(\xi)$ expressed as a linear combination of Hermite polynomials — not as the square of such a polynomial, as is the case with expression (46). The calculation is presented in the Appendix in the more general context of an algebra (the algebra of Hermite polynomials). Substitution of relation (57) into the expression (46) yields the expression for $\rho_n(\xi)$ in the required form:

$$\rho_n(\xi) = \frac{1}{\sqrt{\pi}} \sum_{s=0}^{n} \frac{n!}{s!s!\,(n-s)!2^s} H_{2s}(\xi)\, e^{-\xi^2}. \tag{47}$$

The quantum–mechanical expectation values of a function $f(\xi)$ in position space, is

$$\langle f \rangle_n = \int_{-\infty}^{\infty} \rho_n(\xi)\, f(\xi)\, \mathrm{d}\xi. \tag{48}$$

If we compare this expression with the corresponding expression (41) in classical mechanics, we see that there is a “loss of a variable” in the transition to quantum mechanics. It is as if this theory had a “hidden distribution” $u(\xi, \eta)$ over Φ such that the probability density (47) were given by its partial integral $\int_{-\infty}^{\infty} u(\xi, \eta)\, \mathrm{d}\eta$. We shall see later that this is true for the harmonic oscillator.

4. *Quantum mechanics in phase space*

The abstract algebraic structure $\{\mathcal{H}, \sigma, \alpha\}$ which satisfies the quantum mechanical association identity (11) has the standard Heisenberg representation in terms of Hermitian operators, but it also admits a realization in the phase space of classical mechanics, [1]. To find this realization, we start with the Poisson product ∇, defined by relation (37), and observe that its powers, ∇^n, are also bilinear operators in the space of observables, i.e., if f and g are C^∞ function over the phase space

Φ, so is the function $f\,\nabla^n g$. The powers of ∇ are defined as the formal powers of a binomial expression, i.e.:

$$\nabla^n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} \left(\overleftarrow{\partial}_\eta\right)^{n-k} \left(\overleftarrow{\partial}_\xi\right)^{k} \left(\overrightarrow{\partial}_\eta\right)^{k} \left(\overrightarrow{\partial}_\xi\right)^{n-k} . \tag{49}$$

Consequently, if a function $F(z)$ is defined as a polynomial or Taylor series, the formal expression

$$F(\nabla) = \sum_n \tfrac{1}{n!} \left[f^{(n)}(z)\right]_{z=0} \nabla^n$$

defines a bilinear operator in the space of C^∞ functions in Φ . We can now ask if there exit two analytic functions, one even, $S(z)$, and one odd, $A(z)$, such that the corresponding bilinear operators $S(\nabla)$ and $A(\nabla)$ could be equated with σ and α, respectively, and satisfy the algebraic identities of abstract mechanics. The answer is positive and the solution unique up to a coefficient [1]:

$$\sigma = \cos(c\nabla) , \tag{50}$$

$$\alpha = \frac{1}{c} \sin(c\nabla) . \tag{51}$$

At this point, the coefficient c is an arbitrary dimensionless number. For $c = 0$ we retrieve classical mechanics, for $c \neq 0$ these two products give us the phase space realization of quantum mechanics. The numerical value of c is still arbitrary. It will be determined later from the normalization condition.

This completes the formalism necessary to solve and discuss, in Part II, the quantum mechanical harmonic oscillator in phase space. To get as much insight as possible from this work, we shall solve the problem twice, first in linear coordinates (positions and momenta), and then in "polar-like" coordinates (time and energy). Both approaches lead to the same result in terms of Laguerre polynomials — the second approach directly, the first indirectly through products of Hermite polynomials.

Appendix: The algebra of Hermite polynomials

The product of any two Hermite polynomials is a polynomial, and, hence, a linear combination of other Hermite polynomials. In other words, the Hermite polynomials form an (infinite dimensional) algebra. To exhibit this algebra we have to compute its structure constants, i.e., the numerical coefficients A^r_{nm} in the expansion

$$H_n H_m = \sum_{r \leq n+m} A^r_{nm} H_r . \tag{52}$$

In the sequel we freely use the standard identities for Hermite polynomials, as listed e.g. in Refs. 7 and 8. We first extract A^r_{nm} from this equation with the help of the orthogonality relation for Hermite polynomials by multiplying both sides by $H_s e^{-z^2}$ for arbitrary s, and then integrating over the real line. The result is

$$A^s_{nm} = \frac{1}{\sqrt{\pi}} \frac{1}{2^s s!} \int\limits_{-\infty}^{\infty} H_n H_m H_s e^{-z^2} \mathrm{d}z. \tag{53}$$

To perform the integration we have to reduce the integrand to a product of only two Hermite polynomials. This can be done by repeated partial integrations. The number of integrations will be well defined if we take the lowest order polynomial as the factor function to be integrated. Since the orders n, m, and s are on the same footing in the integrand (even though they are not in the full relation (53)) we may consider any one of them to be minimal. If we assume $s \leq n$, and $s \leq m$, the following suggests itself as a good splitting of the integrand into the form $\int uv' \mathrm{d}z$:

$$\begin{aligned} u &= H_n H_m, \\ v' &= H_s e^{-z^2}. \end{aligned}$$

We can then compute the derivative of u and the integral of v':

$$\begin{aligned} u' &= 2\left(nH_{n-1}H_m + mH_nH_{m-1}\right), \\ v &= -H_{s-1}e^{-z^2} + K_s. \end{aligned}$$

Then,

$$\int\limits_{-\infty}^{\infty} uv' \mathrm{d}z = \left[-H_n H_m H_{s-1} e^{-z^2}\right]_{-\infty}^{\infty} + K_s \left[H_n H_m\right]_{-\infty}^{\infty} - \int\limits_{-\infty}^{\infty} u'v \mathrm{d}z.$$

The first part vanishes identically. The second part is infinite if $n+m$ is odd, which implies that the integration constant K_s must vanish for all values of s. What remains is $\int\limits_{-\infty}^{\infty} uv' \mathrm{d}z = -\int\limits_{-\infty}^{\infty} u'v \mathrm{d}z$, so that repeating the partial integration is straightforward. Clearly, the third factor in the integrand (53) reduces to $H_{s-s} = H_0 = 1$ after s successive integrations. Bypassing the straightforward algebra, the end result is

$$\begin{aligned} &\int\limits_{-\infty}^{\infty} H_n H_m H_s e^{-z^2} \mathrm{d}z \\ &= 2^s \sum_{p=0}^{s} \frac{s!}{p!\,(s-p)!} \frac{n!}{(n-p)!} \frac{m!}{(m-s+p)!} \int\limits_{-\infty}^{\infty} H_{n-p} H_{m-s+p} e^{-z^2} \mathrm{d}z. \end{aligned}$$

Substitution of this expression into relation (53) with the orthogonality relation for Hermite polynomials yields

$$A^s_{nm} = \sum_{p=0}^{s} \frac{n!m!2^{n-p}}{p!\,(s-p)!\,(m-s+p)!}\delta_{n-p,m-s+p}. \tag{54}$$

We see that p is restricted to the value

$$p = (s+n-m)/2.$$

In spite of its apparent half-integer form, p is always an integer. This is due to the fact that Hermite polynomials of even (odd) order have only even (odd) terms, which further implies that s is of the same parity as $(m+n)$. Substitution of the expression for p into relation (54) yields the final expression for the structure constants of the Hermite algebra:

$$A^s_{nm} = \frac{n!m!2^{(n+m-s)/2}}{\left(\frac{s+n-m}{2}\right)!\left(\frac{m+s-n}{2}\right)!\left(\frac{n+m-s}{2}\right)!}. \tag{55}$$

A case of special interest to us is the expression for the squares of Hermite polynomials. By taking $n = m$ and exploiting the consequence that s is even, i.e., by writing $s = 2r$, we obtain the expression

$$A^{2r}_{nn} = \frac{n!n!2^{n-r}}{r!r!\,(n-r)!}, \tag{56}$$

hence

$$(H_n(z))^2 = \sum_{r=0}^{n} \frac{n!n!2^{n-r}}{r!r!\,(n-r)!} H_{2r}(z). \tag{57}$$

This completes the construction of the algebra of Hermite polynomials.

We shall need one additional relation. It is the expression of even Hermite polynomials in the argument $\sqrt{2}z$ in terms of polynomials in the argument z. The computation of this linear expansion will take advantage of the algebra we have just derived.

The starting point is the addition theorem for Hermite polynomials. By taking $n = 2r$ and $z_1 = z_2 = z/\sqrt{2}$, this theorem yields

$$H_{2r}\left(\sqrt{2}z\right) = \frac{1}{2^r}\sum_{k=0}^{2r}\binom{2r}{k} H_k(z)\,H_{2r-k}(z). \tag{58}$$

Since $H_{2r}\left(\sqrt{2}z\right)$ is an even function of z, the products of the polynomials in the sum are also even. This implies that only the even structure constants, $A^{2s}_{k,2r-k}$, enter the expansion. Performing the substitutions, we get

$$H_k\left(z\right)H_{2r-k}\left(z\right)=\sum_{s=0}^{r}\tfrac{k!(2r-k)!2^{r-s}}{(s+k-r)!(s+r-k)!(r-s)!}H_{2s}\left(z\right).$$

This relation, along with (58), yields

$$H_{2r}\left(\sqrt{2}z\right)=\sum_{s=0}^{r}\left[\sum_{k=r-s}^{r+s}\tfrac{1}{(s+k-r)!(s+r-k)!}\right]\tfrac{(2r)!}{(r-s)!2^s}H_{2s}\left(z\right).$$

The expression in square brackets is easily evaluated using the substitution $m=k-r+s$:

$$\sum_{k=r-s}^{r+s}\frac{1}{(s+k-r)!\,(s+r-k)!}$$

$$=\sum_{m=0}^{2s}\frac{1}{m!\,(2s-m)!}=\frac{1}{(2s)!}\sum_{m=0}^{2s}\binom{2s}{m}=\frac{2^{2s}}{(2s)!}.$$

Hence, the desired relation is

$$H_{2r}\left(\sqrt{2}z\right)=\sum_{s=0}^{r}\frac{(2r)!2^s}{(2s)!\,(r-s)!}H_{2s}\left(z\right). \tag{59}$$

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KVANTNI OSCILATOR U FAZNOM PROSTORU

Kvantnu mehaniku je moguće formulirati u istom prostoru u kojem je formulirana klasična mehanika. Razlika među tim teorijama se pojavljuje u algebarskim strukturama realnog linearnog prostora dinamičkih varijabli, a ne u samim varijablama. Dakle, isti se Hamiltonijan može interpretirati ili klasično ili kvantno, što proširuje Bohrov princip korespondencije, koji se sad odnosi na matematske strukture, a ne samo na numerička rješenja. Kvantno–mehanička stanja su realne funkcije u faznom prostoru, analogna gustoći vjerojatnosti u statističkoj mehanici. U prvom dijelu članka razvija se formalizam za rješavanje kvantno–mehaničkih problema u faznom prostoru, specifično harmoničkog oscilatora. U drugom prikazat ćemo egzaktno rješenje i usporedbe sa standardnim pristupom.