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THE QUANTUM OSCILLATOR IN PHASE SPACE. Part II

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Applying the general formalism of quantum mechanics in phase space developed in Part I, we solve the problem of the stationary harmonic oscillator and show that the Hilbert space and phase space solutions are fully consistent.

1. Introduction

In the previous paper [1] (referred to as Part I), we developed the general formalism of quantum mechanics in phase space, starting from an algebraic structure that encapsulates both classical and quantum mechanics. That approach allows a comparative study of foundations of quantum mechanics, as the same physical problem can be treated in independent ways. Comparison of the solutions of classical and quantum mechanics in phase space may offer new insights into the physical problems that are accessible to both approaches.

The simplest, yet one of the most important physical systems is the harmonic oscillator. Due to the fact that its Hamiltonian is of the second order, the problem can be exactly solved in phase space with only moderate effort. This is the objective of the present work.

We take two approaches. One, in terms of Laguerre polynomials, is applicable only to the stationary case. The other, in terms of Hermite polynomials, allows generalization to a harmonically oscillating wave packet (to be presented elsewhere). Finally, we show the complete equivalence of the Hilbert space and phase space solutions where the two can be compared – which is only in the position space.

The additional information contained in the phase space solution may not have physical significance, but helps understand Bohr's correspondence principle from the viewpoint of mathematical structure.

2. The Cartesian approach (Hermite polynomials)

For the Hamiltonian χ given by Eq. (14) of Ref. 1 (hereafter referred as I), the bilinear operators defined by Eqs. (50) and (51) in I generate the following linear operators in $\mathcal{H}$:

$$\begin{aligned}\chi\alpha &= \frac{1}{c}\chi\sin(c\nabla) \\ &= \frac{1}{2}(\xi^2+\eta^2)(\nabla-\frac{1}{3!}c^2\nabla^3+\cdots) \\ &= \eta\partial_\xi-\xi\partial_\eta,\end{aligned} \tag{1}$$

$$\begin{aligned}\chi\sigma &= \chi\cos(c\nabla) \\ &= \frac{1}{2}(\xi^2+\eta^2)(1-\frac{1}{2!}c^2\nabla^2+\frac{1}{4!}c^4\nabla^4\cdots) \\ &= \frac{1}{2}\left(\xi^2-c^2\partial_\xi^2\right)+\frac{1}{2}\left(\eta^2-c^2\partial_\eta^2\right).\end{aligned} \tag{2}$$

We see that the operator (1) of infinitesimal motions is identical to its classical counterpart defined by Eq. (38) in I. This is because χ is a polynomial of only second order, so that derivatives of order higher than two vanish. As for the operator (2), whose expansion stops at the second derivative, it formally happens to be the sum of two Schrödinger operators of the form (42) in I – one for each phase space coordinate.

To simplify calculations, we define new temporary variables, γ,ζ, which absorb the coefficient c:

$$\xi=\sqrt{c}\zeta, \tag{3}$$

$$\eta=\sqrt{c}\gamma. \tag{4}$$

The two linear operators are then

$$\chi\alpha=\gamma\partial_\zeta-\zeta\partial_\gamma, \tag{5}$$

$$\chi\sigma=c\left[\frac{1}{2}\left(\zeta^2-\partial_\zeta^2\right)+\frac{1}{2}\left(\gamma^2-\partial_\gamma^2\right)\right]. \tag{6}$$

The characteristic equation (15) in I now reads

$$\left[\frac{1}{2}\left(\zeta^2-\partial_\zeta^2\right)+\frac{1}{2}\left(\gamma^2-\partial_\gamma^2\right)\right]u_\lambda=\frac{1}{c}\lambda u_\lambda. \tag{7}$$

This differential equation is easily solved by separation of variables. Since each of the variables ζ,γ, leads to eigenfunctions of the form (43) in I, the solution u_λ is a product of such functions. The label λ represents a pair of indices, i.e., $u_\lambda=u_{kl}$. Hence, leaving out the normalization coefficients A_k, A_l, we have

$$u_{kl}\left(\zeta,\gamma\right)=H_k\left(\zeta\right)\mathrm{e}^{-\zeta^2/2}H_l\left(\gamma\right)\mathrm{e}^{-\gamma^2/2}. \tag{8}$$

The eigenvalues are

$$\lambda=\left(m+1\right)c, \tag{9}$$

where $m=k+l$.

The ground state quantum numbers are $k=l=0$, and the ground level energy is $\lambda=c$. Returning to phase space variables by reversing the substitutions (3) and (4), one obtains the following expression for the ground level eigenfunction

$$u_0=K\mathrm{e}^{-\chi/c}. \tag{10}$$

For this function to be a pure state, it must satisfy the idempotence condition (12) in I, which then fixes the value of the coefficient K. To apply this condition, we make the substitution $r=s=-1$ in the general formula (A8). The resulting equation,

$$\mathrm{e}^{-\chi/c}\sigma\mathrm{e}^{-\chi/c}=\frac{1}{2}\mathrm{e}^{-\chi/c}, \tag{11}$$

together with $u_0\sigma u_0=u_0$, implies $K=2$, but still leaves c arbitrary:

$$u_0=2\mathrm{e}^{-\chi/c}. \tag{12}$$

We can now compute the measure–defining constant N. Equations (14) and (35) in I together with Eq. (10) yield the equation:

$$2N\int_\Phi \mathrm{e}^{-(\xi^2+\eta^2)/2c}\mathrm{d}\xi\mathrm{d}\eta=1, \tag{13}$$

which implies the following connection between N and c:

$$Nc=\frac{1}{4\pi}. \tag{14}$$

We now have a choice between two distinguished possibilities. One case is $N=1$, which yields the simple phase space measure $\mathrm{d}\xi\mathrm{d}\eta$, but implies $c=1/4\pi$. This value of c would unnecessarily complicate the state functions. The other distinguished possibility is $c = 1/2$, which implies $N = 1/2\pi$. The advantage of having $c = 1/2$ is that the state u_0 , relation (12), then reads

$$u_0(\xi,\eta) = 2\mathrm{e}^{-\eta^2}\mathrm{e}^{-\xi^2}, \tag{15}$$

which is the same function of ξ as the Schrödinger solution (46) in I for $n = 0$, namely

$$\rho_0(\xi) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{-\xi^2}, \tag{16}$$

while for the choice $c = 1/4\pi$, the comparison requires intermediate coordinate transformations. In addition, if one takes $c = 1/2$, the energy eigenvalues (9) assume their standard form $\lambda = n+1/2$, where $n = m/2$ (provided c is not a function of n — which is true, but remains to be proved). It thus seems that the normalization $N = 1/2\pi$ is computationally preferable, but we shall postpone the decision until we compute the states for the higher energy levels. It is indeed essential to verify that relation (14), derived for $n = 0$, is actually valid for all $n \in \mathbf{N}$.

2.1. The higher energy levels

In the excited states, the quantum number might be considered "degenerate", there being $m+1$ linearly independent eigenfunctions u_{kl} which satisfy the characteristic equation (7). Since the energy levels are not degenerate in Hilbert space quantum mechanics, this is an indication of a potentially instructive difference between the two formulations, but we shall not pursue it here. For a given value of m, the most general phase space eigenfunction is a linear combination

$$u = \sum_{k+l=m} C_{kl}u_{kl} \tag{17}$$

with arbitrary real coefficients C_{kl}. For this eigenfunction to be a stationary state, it must be idempotent, $u\sigma u = u$, and normalized, $\langle u\rangle = 1$. These conditions determine the coefficients. The computation is difficult to perform directly, but simple if we take advantage of the sigma-orthogonality theorem, which states that u is idempotent if it is a constant of the motion, i.e., if $\chi\alpha u = 0$. Applying the operator $\chi\alpha$, defined by relation (5), to the function u, defined by relations (17) and (8), yields

$$\chi\alpha u = \frac{1}{2}\sum_{k+l=m} C_{kl}\left[\gamma H_k'(\zeta)\,H_l(\gamma) - \zeta H_k(\zeta)\,H_l'(\gamma)\right]\mathrm{e}^{-\left(\zeta^2+\gamma^2\right)/2}. \tag{18}$$

With the help of standard identities, we first eliminate from this expression the derivatives of the Hermite polynomials. The resulting equation is

$$\chi\alpha u = \frac{1}{2}\sum_{k+l=m} C_{kl}\left[kH_{k-1}(\zeta)\cdot\gamma H_l(\gamma) - \zeta H_k(\zeta)\cdot lH_{l-1}(\gamma)\right]\mathrm{e}^{-\left(\zeta^2+\gamma^2\right)/2}. \tag{19}$$

We next eliminate the variables γ and ζ which appear as coefficients to the Hermite polynomials:

$$\chi\alpha u = \frac{1}{4}\sum_{k+l=m} C_{kl}\,[kH_{k-1}(\zeta)H_{l+1}(\gamma) - lH_{k+1}(\zeta)H_{l-1}(\gamma)]\,\mathrm{e}^{-(\zeta^2+\gamma^2)/2}. \qquad (20)$$

This result can be rewritten in the compact form

$$\chi\alpha u = \sum_{k+l=m} D_{kl}u_{kl}. \qquad (21)$$

This expression brings out the fact that each $(m+1)$-dimensional sub-space of those eigenfunctions which belong to the same energy eigenvalue is invariant under the group of motions generated by the Hamiltonian. The coefficients D_{kl} are linear combinations of the coefficients C_{kl}:

$$D_{kl} = 2\,[(k+1)\,C_{k+1,l-1} - (l+1)\,C_{k-1,l+1}]\,. \qquad (22)$$

The fixed point of the motion (i.e., the time-independent solution) is then defined by the condition $D_{kl} = 0$, which implies the following system of $m+1$ homogeneous linear equations for the coefficients C_{kl}:

$$(k+1)\,C_{k+1,l-1} = (l+1)\,C_{k-1,l+1}, \qquad (23)$$

where $k+l = m$. To solve this system, we first observe that there is no non–trivial solution if $k+l$ is odd. This can be seen as follows: m single steps in the index k (i.e., $k \to k+1$) are needed to traverse the set of coefficients $\{C_{0,m}, C_{1,m-1}, \cdots, C_{m,0}\}$, but the recursion relation (23) proceeds in double steps (i.e., $k \to k+2$). This implies that m is even. Hence we can write

$$m = 2n \qquad (24)$$

for some n. Similarly, there are no non-trivial solutions if both k and l are odd. To see this, let us consider the first odd coefficient, $C_{1,m-1}$. By relation (23), it is proportional to $C_{-1,m+1}$, a coefficient which does not exist, i.e., equals zero. Recursion by two propagates this value to all odd coefficients. Hence, all non-zero coefficients being of even index, we write $k = 2r$, $l = 2s$, for some r and s, which implies $n = r+s$. The solution of equation (23) then follows as

$$C_{2r,2s} = \frac{C_n}{(2r)!!\,(2s)!!}. \qquad (25)$$

Due to the homogeneity of the system of equations (15), the coefficients C_n are still arbitrary. Hence, up to the factors C_n, the excited states are given by the functions

$$u_n = C_n \sum_{r+s=n} \frac{1}{(2r)!!\,(2s)!!} H_{2r}\,(\zeta)\,\mathrm{e}^{-\zeta^2/2} H_{2s}\,(\gamma)\,\mathrm{e}^{-\gamma^2/2}. \qquad (26)$$

The coefficients C_n could be determined directly from the idempotence condition $u_n\sigma u_n = u_n$, but at great computational cost. Fortunately, they will be found effortlessly later using generating functions. The result is $C_n = 2^{1-n}$.

3. The “polar” approach (Laguerre)

The phase space expression (26) for the excited states of the harmonic oscillator looks like an intuitively acceptable extension of the standard solution, Eq. (47) in I, but it is unduly complicated. This is due to the fact that it describes the rotationally symmetric harmonic oscillator in position and momentum coordinates — a phase space coordinate system which does not reflect the rotational symmetry of the Hamiltonian. A great simplification is achieved if the coordinates ζ, γ, in expression (26), are transformed to the invariant combination $\zeta^2+\gamma^2$. This is done in several steps. First, we use the well–known connection between Hermite and Laguerre polynomials to replace the Hermite polynomials by Laguerre's associated polynomials of index $-1/2$. This yields

$$u_n = C_n 2^n (-1)^n \sum_{r+s=n} L_r^{(-1/2)}(\zeta^2) L_s^{(-1/2)}(\gamma^2). \tag{27}$$

Next, we collect the sum of products of these polynomials with the help of the addition theorem for Hermite polynomials. The result is

$$u_n = C_n\,(-1)^n\,2^n L_n\left(\zeta^2+\gamma^2\right)\mathrm{e}^{-\left(\zeta^2+\gamma^2\right)/2}. \tag{28}$$

Finally, using relations (3) and (4), we transform this function to the original variables, ξ, η. This leads to the compact expression

$$u_n = C_n\,(-1)^n\,2^n L_n\,(2\chi/c)\,\mathrm{e}^{-\chi/c}. \tag{29}$$

We shall now obtain this solution directly, without the intermediate step involving Hermite polynomials. To this end, we make a transformation of phase space coordinates from ξ, η, to χ, τ, and then drop τ, since the system is time independent. When applied to functions of χ only, the differential operators we need are:

$$\begin{aligned}
\partial_\xi &= \xi \frac{d}{\mathrm{d}\chi}, \\
\partial_\eta &= \eta \frac{d}{\mathrm{d}\chi}, \\
\partial_\xi^2 &= \frac{d}{\mathrm{d}\chi} + \xi^2 \frac{d^2}{\mathrm{d}\chi^2}, \\
\partial_\eta^2 &= \frac{d}{\mathrm{d}\chi} + \eta^2 \frac{d^2}{\mathrm{d}\chi^2}.
\end{aligned}$$

These transformations lead to

$$\chi\nabla^2 = \partial_\xi^2 + \partial_\eta^2 = 2\left(\frac{d}{\mathrm{d}\chi} + \chi \frac{d^2}{\mathrm{d}\chi^2}\right). \tag{30}$$

Let us now write the function u in the form

$$u(\chi) = F(r\chi)\, \mathrm{e}^{-s\chi}, \tag{31}$$

where F is the new unknown function and s an unknown parameter. The inessential parameter r is introduced to help bring the resulting differential equation into a recognizable standard form. Substitution of this function and of the operator (30) into the characteristic equation

$$\chi\sigma u = \chi\left(1 - \frac{1}{2}c^2\nabla^2\right)u = \lambda u, \tag{32}$$

yields the following differential equation for F:

$$c^2r^2\chi F'' + c^2r(1-2s\chi)F' + \left(c^2s^2\chi - c^2s + \lambda - \chi\right)F = 0. \tag{33}$$

By selecting the parameters as

$$s = 1/c,$$
$$r = 2s = 2/c,$$
$$\lambda = 2c(n+1/2),$$

and switching to a new variable

$$z = r\chi, \tag{34}$$

which is simply the argument of the function F, the differential equation for F becomes the Laguerre equation, that is

$$zF''(z) + (1-z)F'(z) + nF(z) = 0. \tag{35}$$

Hence, the states u_n are proportional to products of Laguerre polynomials and exponential functions. To compute the unknown coefficients it is convenient to separate them from the functional part. Let us denote the functional part by v_n, i.e.:

$$u_n = K_n v_n, \tag{36}$$

$$v_n = L_n(2\chi/c)\, \mathrm{e}^{-\chi/c}. \tag{37}$$

The values of the coefficients K_n follow from the idempotence requirement for the states u_n — a computation which was postponed when C_n in equation (26) had to be determined. They are now easily computed using generating functions. To this end, we define the generating function $V(w)$ for the sequence of functions v_n, relation (37), as:

$$V(w) = \sum_{n=0}^{\infty} v_n w^n. \tag{38}$$

From relations (37) and the generating function for Laguerre polynomials follows

$$V(w) = \frac{1}{1-w} \exp\left(-\frac{1+w}{1-w}\chi/c\right). \tag{39}$$

Substitution of relation (36) into the idempotence requirement for u_n, yields

$$v_n \sigma v_n = v_n / K_n. \tag{40}$$

While it is difficult to compute the sigma square of v_n directly, we can bypass this step by computing instead the sigma-square of V — which is now straightforward since V is an "invariant exponential" whose σ -algebra is developed in the appendix. Indeed

$$V \sigma V = \frac{1}{(1-w)^2} \exp\left(-\frac{1+w}{1-w}\chi/c\right) \sigma \exp\left(-\frac{1+w}{1-w}\chi/c\right). \tag{41}$$

By taking $r = s = -(1+w)/(1-w)$ in equation (A11), we get

$$V(w)\, \sigma V(w) = \frac{1}{2} \frac{1}{1+w^2} \exp\left(-\frac{1-w^2}{1+w^2}\chi/c\right). \tag{42}$$

Except for the factor $1/2$, this function is the same as the definition of V in relation (39), provided we replace w by $-w^2$. Hence

$$V(w)\, \sigma V(w) = \frac{1}{2} V\left(-w^2\right) = \frac{1}{2} \sum_{n=0}^{\infty} v_n \left(-w^2\right)^n. \tag{43}$$

Independently of this, we also get the following equation from the definition of V, relation (38), and from the orthogonality of states, Eq. (19) in I:

$$V(w)\, \sigma V(w) = \sum_{n=0}^{\infty} \frac{1}{K_n} v_n (w^2)^n. \tag{44}$$

Comparison of relations (43) and (44) yields

$$K_n = 2\,(-1)^n. \tag{45}$$

Hence, the states are

$$u_n = 2\,(-1)^n L_n(2\chi/c)\, \mathrm{e}^{-\chi/c}. \tag{46}$$

This result is functionally identical to the solution (29) obtained by separation of variables, but we have now determined the normalization coefficients as well:

$$C_n = 2^{1-n}. \tag{47}$$

3.1. Completeness

We have shown by abstract arguments that the states u_n are sigma–orthogonal and idempotent up to a factor, Eq. (19) in I. They are normalized (to idempotence) by the proper choice of the coefficients K_n or C_n, equations (45) and (47). To see if they form a complete set, we have to compute their sum — which must be equal to unity for completeness. To this end, we construct a generating function $U(w)$ for the states according to the definition

$$U(w) = \sum_{n=0}^{\infty} u_n w^n. \tag{48}$$

Its usefulness for the problem at hand stems from the fact that if we take $w = 1$ we get $U(1) = \sum_{n=0}^{\infty} u_n$, which is the sum we have to compute. Comparison of expression (48) with the generating function for the intermediate functions v_n, relations (38) and (45), yields

$$U(w) = 2V(-w), \tag{49}$$

or, explicitly

$$U(w) = \frac{2}{1+w} \exp\left(-\frac{1-w}{1+w}\chi/c\right). \tag{50}$$

By taking $w = 1$ we indeed get $U(1) = 1$, which proves that the set of eigenfunctions u_n is complete.

3.2. Trace normalization

We note that all results obtained so far are valid for any value of the coefficient c which appears in the definition $\sigma = \cos(c\nabla)$ of the Jordan product, but we still have to satisfy the unit trace condition $\langle u_n \rangle = 1$, defined by Eq. (35) in I. The integration is most conveniently done in polar coordinates, where $R^2 = 2\chi$. The dimensionless phase space measure is then

$$N\mathrm{d}\xi\mathrm{d}\eta = NR\mathrm{d}R\mathrm{d}\phi = N\mathrm{d}\chi\mathrm{d}\phi.$$

For any function f of χ alone, this implies

$$\langle f \rangle = N \int_{\Phi} \mathrm{d}\xi\mathrm{d}\eta\, f(\chi) = 2\pi N \int_0^{\infty} f(\chi)\,\mathrm{d}\chi. \tag{51}$$

To compute the value of c, we note that of the two expressions for the generating function U, (48) and (50), only one contains c explicitly. Hence, by computing the trace $\langle U \rangle$ of both and equating the results we get an equation for c. Thus, relation (48), with $\langle u_n \rangle = 1$, yields

$$\langle U \rangle = \sum_{n=0}^{\infty} w^n = \frac{1}{1-w}, \tag{52}$$

while relation (50) together with (51) leads to

$$\langle U \rangle = \frac{4\pi}{1+w} N \int_0^\infty \mathrm{e}^{-\frac{1-w}{1+w}\chi/c} \mathrm{d}\chi = 4\pi c \frac{1}{1-w} N \tag{53}$$

for the trace in polar coordinates. Comparison of the two results yields $4\pi cN = 1$, which is the same equation as (14). This proves that the relationship between the measure-defining coefficient N and the coefficient c of the operator ∇ is the same for all energy levels n. As indicated earlier, we select

$$c = \frac{1}{2}, \tag{54}$$

$$N = \frac{1}{2\pi}. \tag{55}$$

The sigma–orthogonality relation, Eq. (19) in I, now reads

$$u_m \sigma u_n = u_n \delta_{mn}. \tag{56}$$

3.3. The collected analytic results

Relations (26), (54), (3), (4) and (47) yield the following expression for the states in terms of Hermite polynomials:

$$u_n = \frac{2}{2^{2n}} \sum_{r+s=n} \frac{1}{r!s!} H_{2r}\left(\sqrt{2}\xi\right) \mathrm{e}^{-\xi^2} H_{2s}\left(\sqrt{2}\eta\right) \mathrm{e}^{-\eta^2}. \tag{57}$$

Relations (46) and (54) yield the following expression for the same states in terms of Laguerre polynomials:

$$u_n = 2\,(-1)^n L_n\,(4\chi)\,\mathrm{e}^{-2\chi}. \tag{58}$$

Relations (9), (54), and (24) yield the energy levels:

$$\lambda = n + 1/2. \tag{59}$$

Relation (58) yields the generating function $G(w,z)$ for the states:

$$G(w,\chi) \equiv \sum_{n=0}^{\infty} u_n(\chi) w^n = \frac{2}{1+w} \mathrm{e}^{-2(1-w)\chi/(1+w)}. \tag{60}$$

3.4. Separation of variables

The expression (57) for u_n is a sum of products of functions of a single variable. To bring out this fact, we define the following sequence of functions of a single real variable, z:

$$Q_k(z) = \frac{\sqrt{2}}{2^{2k}k!} H_{2k}(\sqrt{2}z)\mathrm{e}^{-z^2}. \tag{61}$$

The idempotents u_n, given by relation (57), now read:

$$u_n(\xi,\eta) = \sum_{r+s=n} Q_r(\xi)Q_s(\eta). \tag{62}$$

Since one of the objectives of the present work is to compare the two formulations of quantum mechanics (in Hilbert space and in phase space), the state (57), which is of phase space origin, is to be compared with the state (see Eq. (47) in I), which is of Hilbert space origin. The functional difference in the variable ξ between these two expressions is in the arguments of the Hermite polynomials. To equate these arguments, we have to eliminate the coefficient $\sqrt{2}$ from the argument in expression (61). This is done using relation (58) in I. The new expression for $Q_k(z)$,

$$Q_k(z) = \frac{\sqrt{2}}{2^{2k}k!} \sum_{l=0}^{k} \frac{(2k)!2^l}{(2l)!(k-l)!} H_{2l}(z)\mathrm{e}^{-z^2}, \tag{63}$$

is now of the right form for the comparison in question. Since the standard quantum mechanical probability density given by Eq. (47) in I is a function of ξ alone, the variable η remains to be eliminated from the state $u_n(\xi,\eta)$. This will be done by integration in the next section.

3.5. Orthogonality

The states u_n have another important property: they are orthogonal with respect to the scalar product of functions which is defined by integration over phase space. To prove this, we substitute $u_n \cdot u_m$ for f in relation (51). Since $N = 1/2\pi$, this yields

$$T(u_n \cdot u_m) = \int_0^\infty u_n \cdot u_m \mathrm{d}\chi. \tag{64}$$

Substitution of the Laguerre expression (58) for the states yields an integral which can be computed using the orthogonality relations for Laguerre polynomials. The result is

$$T(u_n \cdot u_m) = \delta_{nm}. \tag{65}$$

On the other hand, relation (56) implies

$$T(u_n \sigma u_m) = T(u_n)\delta_{nm} = \delta_{nm}, \tag{66}$$

and, hence

$$T(u_n \sigma u_m) = T(u_n \cdot u_m) = \delta_{nm}. \tag{67}$$

It is remarkable that the standard scalar product, $T(u_n \cdot u_m)$, which is not manifestly structural (the ordinary multiplication of functions is not a quantum mechanical structure), is nevertheless a structure. Hence, one could say that the structure-offending part of the integrand $u_n \cdot u_m$ is cancelled by integration.

4. Relationship to Hilbert space

In Hilbert space quantum mechanics, states are represented by wave functions, $\psi(\xi)$. These are complex numbers with no direct experimental interpretation. The connection with measurements is established by the postulate that the probability of observing in the interval $\xi + \mathrm{d}\xi$ a particle whose state vector is $\psi(\xi)$ is given by $\psi\bar{\psi}\mathrm{d}\xi$. Hence, $\rho(\xi) = \psi(\xi)\bar{\psi}(\xi)$ is a probability density in position space, provided $\psi(\xi)$ is normalized, i.e., $\int\limits_{-\infty}^{\infty} \rho(\xi)\mathrm{d}\xi = 1$.

In phase space quantum mechanics, states are represented by real C^∞ functions, $u(\xi,\eta)$, which are σ-idempotent, $u\sigma u = u$, and normalized, $\frac{1}{2\pi}\int\limits_{\Phi} u(\xi,\eta)\mathrm{d}\xi\mathrm{d}\eta = 1$. Under the integral sign, the functions u behave like probability densities: the expectation value of an observable f in the state u is $\langle f\rangle_u = \frac{1}{2\pi}\int\limits_{\Phi} f(\xi,\eta)\cdot u(\xi,\eta)\mathrm{d}\xi\mathrm{d}\eta$, just as in classical mechanics. The difference with classical mechanics is that the quantum mechanical functions $u(\xi,\eta)$ *are not everywhere non-negative* in phase space. Hence, they are not standard probability densities. This is almost to be expected, since a positive definite probability density in phase space would contradict Heisenberg's uncertainty principle by allowing position and momentum to be specified with arbitrary accuracy.

To find the connection between $\rho(\xi)$ and $u(\xi,\eta)$, let us consider a test observable, f, which is a function of ξ alone, i.e., $f = f(\xi)$. Its expectation value in a state ρ in position space is then

$$\langle f\rangle_\rho = \int\limits_{-\infty}^{\infty} f(\xi)\rho(\xi)\mathrm{d}\xi. \tag{68}$$

In a state u in phase space, the expectation value is

$$\langle f\rangle_u = \frac{1}{2\pi}\int\limits_{\Phi} f(\xi)u(\xi,\eta)\mathrm{d}\xi\mathrm{d}\eta. \tag{69}$$

These numbers will coincide for all f if the following condition holds:

$$\rho(\xi) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} u(\xi,\eta)\mathrm{d}\eta. \tag{70}$$

We can now formulate the conjecture that relates the two realizations of states:

Conjecture. The Equivalence Conjecture. *If* $\psi(\xi)$ *is the Hilbert space state function of a bound and time independent system, and if* $u(\xi,\eta)$ *is the phase space realization of the same state, then*

$$\psi(\xi)\bar{\psi}(\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} u(\xi,\eta)\mathrm{d}\eta. \tag{71}$$

Clearly, for this relation to be applicable, it must be possible to solve in principle, or at least to write down, the two characteristic equations, $\hat{\chi}\psi = E\psi$ and $\chi\sigma u = Eu$, but the phase space and Hilbert space approaches are not necessarily equivalent for unphysical problems. The reason is that while the characteristic equation $\chi\sigma u = \lambda u$ is uniquely defined for any phase space function χ, regardless of whether or not it can be solved, the operator $\hat{\chi}$ is not uniquely defined by the Schrödinger quantization procedure because ξ and $\mathrm{i}\partial_\xi$ do not commute. Consequently, ordering of variables is relevant and there is no unique Schrödinger equation for an arbitrary observable χ.

We shall now verify the conjecture for the harmonic oscillator — upgrading it to the status of theorem in this particular case. To this end, we compute $\rho(\xi)$ from the wave function $\psi(\xi)$, given by relation Eq. (43) in I, and from the idempotent $u(\xi,\eta)$, given by Eq. (57). Since the first part of the computation has already been done, Eq. (47) in I, we turn to the integration of u.

The expression for u best suited for this calculation is given by relations (62) and (61), which, with relation (70), yield

$$\rho(\xi) = \sum_{r+s=n} q_s Q_r(\xi). \tag{72}$$

The coefficients q_s are defined by integration over η:

$$q_s = \frac{1}{2\pi}\int_{-\infty}^{\infty} Q_s(\eta)\mathrm{d}\eta. \tag{73}$$

To compute them, we first substitute a new variable, z, for $\sqrt{2}\eta$:

$$\begin{aligned} q_s &= \frac{1}{2\pi}\frac{\sqrt{2}}{2^{2s}s!}\int_{-\infty}^{\infty} H_{2s}(\sqrt{2}\eta)\mathrm{e}^{-\eta^2}\mathrm{d}\eta \\ &= \frac{1}{2\pi}\frac{1}{2^{2s}s!}\int_{-\infty}^{\infty} H_{2s}(z)\mathrm{e}^{-z^2/2}\mathrm{d}z. \end{aligned}$$

This last expression can be evaluated using the explicit definition of the Hermite polynomials, which, for $n = 2s$ reads:

$$H_{2s}(z) = (2s)!2^{2s}\sum_{m=0}^{s}\frac{(-1)^m}{2^{2m}m!(2s-2m)!}z^{2s-2m}. \tag{74}$$

Writing $m = s - k$, and then substituting this expression into the previous one, yields

$$q_s = \frac{1}{2\pi} \frac{(2s)!(-1)^s}{2^{2s} s!} \sum_{k=0}^{s} \frac{(-1)^k 2^{2k}}{(s-k)!(2k)!} \int_{-\infty}^{\infty} z^{2k} \mathrm{e}^{-z^2/2} \mathrm{d}z. \tag{75}$$

The integral, which represents Gaussian moments M_{2k}, is computed by recursion:

$$M_{2k} = \int_{-\infty}^{\infty} z^{2k} \mathrm{e}^{-z^2/2} \mathrm{d}z = \frac{(2k)!}{2^k k!} \sqrt{2\pi}. \tag{76}$$

Collecting these expressions, one obtains

$$\begin{aligned} q_s &= \tfrac{1}{2\pi} \tfrac{(2s)!(-1)^s}{2^{2s} s!} \textstyle\sum_{k=0}^{s} \tfrac{(-1)^k 2^{2k}}{(s-k)!(2k)!} M_{2k} \\ &= \tfrac{1}{\sqrt{2\pi}} \tfrac{(2s)!(-1)^s}{2^{2s} s!} \textstyle\sum_{k=0}^{s} \tfrac{2^k (-1)^k}{(s-k)! k!} \\ &= \tfrac{1}{\sqrt{2\pi}} \tfrac{(2s)!(-1)^s}{2^{2s} s! s!} \textstyle\sum_{k=0}^{s} \binom{s}{k} (-2)^k \\ &= \tfrac{1}{\sqrt{2\pi}} \tfrac{(2s)!}{2^{2s} s! s!}. \end{aligned} \tag{77}$$

Since the states are of unit trace, relation (72) implies

$$\sum_{r=0}^{n} q_r \int_{-\infty}^{\infty} Q_{n-r}(\xi) \mathrm{d}\xi = 1, \tag{78}$$

which yields:

$$\frac{1}{2^{2n}} \sum_{r+s=n} \frac{(2r)!(2s)!}{r! r! s! s!} = 1. \tag{79}$$

This relation is a consequence of the equivalence conjecture for the harmonic oscillator, but, being an algebraic proposition in its own right, it is either true or false — and hence a test for the conjecture. As we shall see later, it is a special case of the more general relation (87), but it can easily be proved by itself. To this end, we note that it suggests the multiplication rule for the coefficients of power series. To exploit this observation, we define the following power series

$$f(z) = \sum_{r=0}^{\infty} \frac{(2r)!}{r! r! 4^r} z^r, \tag{80}$$

in some appropriate disc of convergence. If relation (79) is true, all coefficients of this series squared are unity:

$$(f(z))^2 = \sum_{n=0}^{\infty} z^n. \tag{81}$$

In the unit disc $|z| < 1$, this yields the closed form

$$f(z) = \frac{1}{\sqrt{1-z}}, \tag{82}$$

whose Taylor expansion

$$f(z) = \sum_{r=0}^{\infty} \frac{1}{r!} \frac{(2r-1)!!}{2^2} z^r \tag{83}$$

is identical to the expression (80), thus verifying equation (79).

The next step is to compare the probability distribution $\rho(\xi)$, obtained from the Hilbert space solution (see Eq. (47) in I) with the phase space solution (72). Combining relations (63), (72) and (77), we obtain the following expression for ρ:

$$\rho(\xi) = \frac{1}{\sqrt{2\pi}} \sum_{r=0}^{n} \frac{\sqrt{2}(2n-2r)!(2r)!}{2^{2n} r!(n-r)!(n-r)!} \sum_{s=0}^{r} \frac{2^s}{(2s)!(r-s)!} H_{2s}(\xi) \mathrm{e}^{-\xi^2}. \tag{84}$$

For comparison with relation (47) in I we shall need an expression whose outer sum over the index s of the Hermite polynomials runs from 0 to n. One obtains it by interchanging the order of summation:

$$\rho(\xi) = \frac{1}{\sqrt{\pi}} \sum_{s=0}^{n} \frac{2^s}{2^{2n}(2s)!} \sum_{r=s}^{n} \frac{(2n-2r)!(2r)!}{r!(n-r)!(n-r)!(r-s)!} H_{2s}(\xi) \mathrm{e}^{-\xi^2}. \tag{85}$$

By the equivalence conjecture, this function should be the same as the function given by expression (47) in I. Since, in both expressions, the functional parts (Hermite polynomials times exponential) and the outer summation have already been brought to the same form, only the following condition on the coefficients remains to be satisfied:

$$\frac{n!}{s!s!(n-s)!2^s} = \frac{2^s}{2^{2n}(2s)!} \sum_{r=s}^{n} \frac{(2n-2r)!(2r)!}{r!(n-r)!(n-r)!(r-s)!}. \tag{86}$$

This is a proposition in two variables, n and s. We cannot "require" that it be true. Like relation (79), it either is or is not.

To bring this combinatorial relation to a more manageable form, we make the following substitutions:

$$q = n - r,$$
$$m = n - s,$$

which imply

$$r = n + q,$$
$$r - s = m - q,$$
$$\sum_{r=s}^{n} = \sum_{q=0}^{m}.$$

Equation (86) now becomes

$$\frac{2^{2m}n!(2(n-m))!}{(n-m)!(n-m)!m!} = \sum_{q=0}^{m} \frac{(2q)!(2(n-q))!}{q!q!(n-q)!(m-q)!}. \tag{87}$$

To prove this relation[1], we first perform the summation on the right-hand side by using hypergeometric functions as a stepping stone. The property of these functions which is relevant here is that they can be written in two ways: as an infinite sum of terms involving Pochhammer symbols, or as a single rational expression involving gamma functions [2]. The basic formulae we shall need are

$$F(a,b;c;z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n n!} z^n, \tag{88}$$

where $c \neq 0, -1, -2, ...$, and

$$F(a,b;c;z) = \frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)}, \tag{89}$$

where $c \neq 0, -1, -2, ...$, and $\mathrm{Re}c > \mathrm{Re}(a+b)$. The definition of the Pochhammer symbols is

$$(a)_n = \frac{\Gamma(n+a)}{\Gamma(a)}. \tag{90}$$

We shall also need the duplication formula for gamma functions,

$$\Gamma(2z) = 2^{2z-1} \frac{\Gamma\left(z+\frac{1}{2}\right)\Gamma(z)}{\Gamma\left(\frac{1}{2}\right)}, \tag{91}$$

and the reciprocity formula

$$\Gamma(z)\,\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}. \tag{92}$$

To write the summand in relation (87) in terms of Pochhammer symbols, we apply twice the duplication formula:

$$\frac{(2q)!}{q!} = \frac{\Gamma(2q+1)}{\Gamma(q+1)}$$

$$= 2^{2q} \frac{\Gamma\left(q+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} = 2^{2q} \left(\frac{1}{2}\right)_q,$$

[1] The proof has been supplied by Professor W. Rühl. We most gratefully acknowledge the contribution.

and

$$\frac{(2\,(n-q))!}{(n-q)!} = 2^{2n-2q}\frac{\Gamma\left(n-q+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}. \tag{93}$$

Substitution of these expressions into relation (87) yields

$$\frac{2^{2m}n!(2(n-m))!}{(n-m)!(n-m)!m!} = 2^{2n}\sum_{q=0}^{m}\frac{\Gamma\left(n-q+\frac{1}{2}\right)\left(\frac{1}{2}\right)_q}{\Gamma\left(\frac{1}{2}\right)q!(m-q)!} \tag{94}$$

The next transformation is

$$\frac{\Gamma\left(n-q+\frac{1}{2}\right)}{(m-q)!} = \frac{\Gamma\left(n+\frac{1}{2}\right)}{m!}\cdot\frac{(-m)_q}{\left(\frac{1}{2}-n\right)_q}, \tag{95}$$

which, with relation (94), yields

$$\frac{2^{2m}n!(2(n-m))!}{(n-m)!(n-m)!} = 2^{2n}\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}\sum_{q=0}^{m}\frac{\left(\frac{1}{2}\right)_q(-m)_q}{q!\left(\frac{1}{2}-n\right)_q} \tag{96}$$

By formula (88), the sum is a hypergeometric function

$$\sum_{q=0}^{\infty}\frac{\left(\frac{1}{2}\right)_q(-m)_q}{q!\left(\frac{1}{2}-n\right)_q} = F\left(\frac{1}{2},-m;\frac{1}{2}-n;1\right). \tag{97}$$

The summation limit in relation (94) is m, but it can be formally taken as ∞ since it stops at m due to the identity $(-m)_m = 0$. By relation (89), the same hypergeometric function can be written in terms of gamma functions:

$$F\left(\frac{1}{2},-m;\frac{1}{2}-n;1\right) = \frac{\Gamma\left(\frac{1}{2}-n\right)\Gamma(-n+m)}{\Gamma(-n)\,\Gamma\left(\frac{1}{2}-n+m\right)}. \tag{98}$$

Since $n > m$, both being natural numbers, the fraction is of the indefinite form ∞/∞. To evaluate it, let us treat n as a complex number $n = z \notin \mathbf{N}$. Applying the reciprocity theorem (92) to the four gamma functions, one obtains the relation

$$F\left(\frac{1}{2},-m;\frac{1}{2}-n;1\right) = \frac{\Gamma(z+1)\,\Gamma\left(\frac{1}{2}+z-m\right)}{\Gamma\left(\frac{1}{2}+z\right)\Gamma(z-m+1)}\cdot S, \tag{99}$$

where

$$\begin{aligned} S &= \frac{\sin(z\pi)\sin\left(\left(\frac{1}{2}-z+m\right)\pi\right)}{\sin\left(\left(\frac{1}{2}-z\right)\pi\right)\sin((z-m)\pi)} \\ &= \frac{\sin(z\pi)\cos((z-m)\pi)}{\cos(z\pi)\sin((z-m)\pi)} = 1. \end{aligned}$$

By continuity, $S=1$ for $z\in\mathbf{N}$ also. Substitution of expressions (97), (98) and (99) into relation (96) yields

$$\frac{(2(n-m))!}{(n-m)!}=2^{2n-2m}\frac{\Gamma\left(\frac{1}{2}+n-m\right)}{\Gamma\left(\frac{1}{2}\right)}. \tag{100}$$

This relation is identically true, since it is the same as (97) with $q=m$. This completes the proof of relation (87). Hence, for the harmonic oscillator at least, the equivalence conjecture is a theorem. Note: Relation (79) is the special case of (87) for $m=n$.

Appendix: The Jordan product of exponentials

Since special cases of the Jordan product of invariant exponentials appear in several proofs in the main text, it is most expedient to derive the general expression only once. The Lie product of such exponentials obviously vanishes identically.

By "invariant exponential" we mean an exponential function of the Hamiltonian, i.e., $u = \mathrm{e}^{a\chi}$, where $\chi = (\xi^2 + \eta^2)$, and a is any real number. The Jordan product $\mathrm{e}^{a\chi}\sigma\mathrm{e}^{b\chi}$ is then the real part of the complex product

$$Y = \mathrm{e}^{a\chi}\mathrm{e}^{\mathrm{i}c\nabla}\mathrm{e}^{b\chi}, \tag{A1}$$

but since the imaginary part of Y (i.e., the Lie product) vanishes, the Jordan product is effectively equal to this expression. By substituting the expressions for χ and for ∇, into relation (A1), one obtains

$$Y = \mathrm{e}^{a\xi^2/2}\mathrm{e}^{a\eta^2/2}\mathrm{e}^{\mathrm{i}c\overleftarrow{\partial}_\eta\overrightarrow{\partial}_\xi}\mathrm{e}^{\mathrm{i}c\overleftarrow{\partial}_\xi\overrightarrow{\partial}_\eta}\mathrm{e}^{b\xi^2/2}\mathrm{e}^{b\eta^2/2}. \tag{A2}$$

An operator of the form $\mathrm{e}^{t\overrightarrow{\partial}_\xi}$ represents a translation by a value t, i.e., $\mathrm{e}^{t\overrightarrow{\partial}_\xi} f(\xi) = f(\xi + t)$. We shall formally preserve this interpretation even if t is not a variable but an operator, provided it commutes with the argument of the function f. Thus:

$$f(\eta)\,\mathrm{e}^{\mathrm{i}c\overleftarrow{\partial}_\eta\overrightarrow{\partial}_\xi} = f\left(\eta + \mathrm{i}c\overrightarrow{\partial}_\xi\right),$$

since $\frac{\partial f}{\partial \xi} = 0$. With this generalization of the concept of displacement, relation (A1) becomes

$$Y = \mathrm{e}^{a\xi^2/2}\mathrm{e}^{\frac{a}{2}\left(\eta + \mathrm{i}c\overrightarrow{\partial}_\xi\right)^2}\mathrm{e}^{\frac{b}{2}\left(\eta - \mathrm{i}c\overleftarrow{\partial}_\xi\right)^2}\mathrm{e}^{b\xi^2/2}.$$

In this expression, the first operator (i.e., the second exponential factor) acts to the right, thus affecting only the last factor. Similarly, the second operator acts only on the first factor. Hence, the expression for Y simplifies to a product of two simpler functions of two variables:

$$Y = \left(\mathrm{e}^{\frac{b}{2}\left(\eta - \mathrm{i}c\partial_\xi\right)^2}\mathrm{e}^{a\xi^2/2}\right)\left(\mathrm{e}^{\frac{a}{2}\left(\eta + \mathrm{i}c\partial_\xi\right)^2}\mathrm{e}^{b\xi^2/2}\right). \tag{A3}$$

Defining a new function

$$P(a,b) = \left(\mathrm{e}^{\frac{a}{2}\left(\eta + \mathrm{i}c\partial_\xi\right)^2}\mathrm{e}^{b\xi^2/2}\right), \tag{A4}$$

of the parameters a, b (the variables ξ, η being assumed,) we obtain

$$Y = P(a,b)\overline{P}(b,a). \tag{A5}$$

Let us compute $P(a,b)$:

$$P(a,b) = \mathrm{e}^{\frac{a}{2}\eta^2}\mathrm{e}^{iac\eta\partial_\xi}\mathrm{e}^{-\frac{a}{2}c^2\partial_\xi^2}\mathrm{e}^{b\xi^2/2}. \tag{A6}$$

We have here a diffusion operator, $\mathrm{e}^{\frac{a}{2}c^2\partial_\xi^2}$, acting on a Gaussian function, $\mathrm{e}^{b\xi^2/2}$, followed by a translation $\mathrm{e}^{\mathrm{i}ac\eta\partial_\xi}$. Since a Gaussian diffuses into a Gaussian, we have, in general

$$\mathrm{e}^{t\partial_x^2}\mathrm{e}^{Cx^2} = A\mathrm{e}^{Bx^2},$$

where C is a constant and A and B are functions of t with initial conditions $A(0) = 1$, $B(0) = C$. Since the left side satisfies the diffusion equation $\partial_t = \partial_x^2$, so must the right side, implying the following differential identity in x:

$$\frac{A'}{A} + B'x^2 = 2B + 4B^2x^2.$$

The solutions which satisfy the initial conditions are

$$B = \frac{C}{1-4Ct},$$

$$A = \frac{1}{\sqrt{1-4Ct}}.$$

We obtain $P(a,b)$ by taking $t = -ac^2/2$, $C = b/2$. With these substitutions, relation (A6) now reads

$$P(a,b) = \frac{1}{\sqrt{abc^2+1}}\mathrm{e}^{\frac{a}{2}\eta^2}\left(\mathrm{e}^{\mathrm{i}ac\eta\partial_\xi}\mathrm{e}^{\frac{1}{2}\frac{b}{abc^2+1}\xi^2}\right).$$

The remaining exponential operator represents a translations in ξ by $\mathrm{i}ac\eta$. Hence:

$$P(a,b) = \frac{1}{\sqrt{abc^2+1}}\mathrm{e}^{-\frac{a}{2}\eta^2}\mathrm{e}^{\frac{1}{2}\frac{b}{abc^2+1}(\xi^2-a^2c^2\eta^2+\mathrm{i}2ac\xi\eta)}. \tag{A7}$$

From (A1), (A5) and (A7) follows the desired relation

$$\mathrm{e}^{a\chi}\sigma\mathrm{e}^{b\chi} = \frac{1}{abc^2+1}\mathrm{e}^{\frac{a+b}{abc^2+1}\chi},$$

which we can simplify by subsumming the universal constant c in new parameters, r and s, defined as $r = ac$, $s = bc$:

$$\mathrm{e}^{r\chi/c}\sigma\mathrm{e}^{s\chi/c} = \frac{1}{rs+1}\mathrm{e}^{\frac{r+s}{rs+1}\chi/c}. \tag{A8}$$

Since $c = 1/2$, we finally get

$$e^{2r\chi}\sigma e^{2s\chi} = \frac{1}{rs+1} e^{2\frac{r+s}{rs+1}\chi}. \tag{A9}$$

It is interesting to note that the exponential coefficient $\frac{r+s}{rs+1}$ has the functional form of the addition theorem for the hyperbolic tangens. To see where this observation might lead, let us write r and s in terms of new parameters, ϕ, ψ, according to the substitution

$$r = \tanh\phi,$$

$$s = \tanh\psi.$$

Relation (A9) now reads

$$e^{2\tanh\phi\chi}\sigma e^{2\tanh\psi\chi} = \frac{\tanh(\phi+\psi)}{\tanh\phi+\tanh\psi} e^{2\tanh(\phi+\psi)\chi}. \tag{A10}$$

Since

$$\frac{\tanh(\phi+\psi)}{\tanh\phi+\tanh\psi} = \frac{\cosh\phi\cosh\psi}{\cosh(\phi+\psi)},$$

we can rewrite relation (A10) as

$$\left(\frac{e^{2\tanh\phi\chi}}{\cosh\phi}\right)\sigma\left(\frac{e^{2\tanh\psi\chi}}{\cosh\psi}\right) = \frac{e^{2\tanh(\phi+\psi)\chi}}{\cosh(\phi+\psi)}.$$

This suggests the definition of a new observable, E, which would be a function of $\phi\chi$ (or simply as a function of ϕ, since the Hamiltonian χ is fixed):

$$E(\phi) = \frac{\exp((2\tanh\phi)\chi)}{\cosh\phi}. \tag{$A11$}$$

What distinguishes this function is that it satisfies the addition theorem:

$$E(\phi)\,\sigma E(\psi) = E(\phi+\psi). \tag{A12}$$

We shall call it the *sigma-exponential function*, as it plays, with respect to σ, the role the ordinary exponential function plays with respect to the ordinary product: they both establish an isomorphic mapping between the multiplicative and additive structures of their respective algebras.

References

1) E. Grgin and G. Sandri, Fizika B **5** (1996) 141;

2) H. Bateman, *High Transcedental Functions I*, Mc Graw Hill Book Company, Inc, 1953.

KVANTNI OSCILATOR U FAZNOM PROSTORU. II DIO

Primjenom općeg formalizma koji je razvijen u I. dijelu rada, riješili smo problem stacionarnog harmoničkog oscilatora i pokazali da su rješenja u Hilbertovom prostoru i fazno–prostorna rješenja potpuno skladna.