# Wigner-Weyl Quantization in the Phase Space Formulation

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Starting from analogies of quantum-classical correspondence, we define desired properties of a quantization scheme between classical functions in phase space and Hermitian operators in a Hilbert space. Motivated by reducing ambiguity, we construct the Wigner-Weyl transforms which produce a quantum algebra corresponding, in the classical limit, to the Poisson algebra. Considering the density operator, we develop the Wigner function, a probability density in phase space describing our system without reference to an ambient Hilbert space. We further specify applications of this quantization technique to coherence and decoherence as they relate to recovering semiclassical behavior.

#### I. INTRODUCTION

In learning quantum mechanics, many of our choices are motivated by the desire for classical intuition to hold. Starting from wave mechanics for example, we use a particular operator representation for position q and momentum p yet even for as simple of an expression as qp, we have ambiguity in how to construct a corresponding Hermitian operator. Once formalizing classical mechanics, we arrive at a number of compounding desires for such a prescription which no quantization can fulfil. As a result, instead of constructing a perfect system of quantization, we instead ask what a particular quantization allows us to understand.

### **II. CLASSICAL FORMALISM**

To tell how well our quantization compares to classical mechanics, we will need to treat it formally. For this, we will begin with the well-known Hamiltonian formalism for a system with N degrees of freedom. Here, the state of our system is described by pairs of coordinates  $q_i$  and  $p_i$  where the index i spans the N degrees of freedom. These correspond to the familiar generalized coordinates and generalized momenta in Lagrangian mechanics. For simplicity, we will assume our coordinates are unbounded. Otherwise, the following arguments hold only locally in so-called Darboux coordinates on a symplectic manifold.

When we speak of a phase space, we mean the space of all possible choices of  $q_i$  and  $p_i$  which we assume live on a smooth symplectic manifold M. For our purposes, we will think of this manifold as  $\mathbb{R}^{2N}$ . We will now consider the space of all real smooth functions on M which we denote  $C^{\infty}(M)$ . To represent our physical system, we fix a particular function, the Hamiltonian,  $H(q_i, p_i, t)$ . Once chosen, the trajectory of a particle is described by the familiar Hamilton's equations of motion:

$$\frac{\partial q_i}{\partial t} = \frac{\partial H}{\partial p_i}$$

$$\frac{\partial p_i}{\partial t} = -\frac{\partial H}{\partial q_i}$$
(1)

From here, we will construct the classical Poisson bracket, a map from two functions  $A, B \in C^{\infty}(M)$  to another denoted  $\{A, B\} \in C^{\infty}(M)$  given by

$$\{A,B\} = \frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q}.$$
 (2)

One particularly useful consequence arises from considering the Poisson bracket of an arbitrary time-independent function with the Hamiltonian. Substituting Hamilton's equations of motion, 1 above, we have

$$\{A, H\} = \frac{\partial A}{\partial q} \frac{\partial q}{\partial t} + \frac{\partial A}{\partial p} \frac{\partial p}{\partial t} = \frac{dA}{dt}$$
(3)

which is why we say the Hamiltonian is the generator of time evolution, even classically. If  $\{A, H\} = 0$ , we say the functions Poisson commute or are in involution. One consequence is that the value of A is conserved along the trajectory so we think of the Poisson bracket as encoding our conserved quantities.

To see why the Poisson bracket is so useful, let us consider a different interpretation. First, we may associate to any function  $A \in C^{\infty}(M)$ , a vector field  $v_A : M \to \mathbb{R}^{2N}$ which assigns to each point  $(q_i, p_i) \in M$  the corresponding trajectory, 1, if we had treated it as a Hamiltonian. That is

$$v_A(q,p) = \sum_{i=1}^{N} \frac{\partial A}{\partial p_i} \hat{q}_i - \frac{\partial A}{\partial q_i} \hat{p}_i, \qquad (4)$$

where hats indicate basis vectors in the space  $\mathbb{R}^{2N}$ . From here, we see that the Poisson bracket may also be interpreted as a directional derivative, that is  $\{A, H\} = v_H \cdot \nabla A = -v_A \cdot \nabla H$ . We further see that if A Poisson commutes with H, that H is unchanging along the trajectory generated by A. This is known as Noether's Theorem, a fundamental law relating symmetries to conserved quantities, which we see is encoded in our Poisson bracket. [1]

In quantum mechanics, we recall the quantum analogue of equation 3 above, the Ehrenfest Theorem which governs the rate of change of expectation values,

$$\frac{d\langle A\rangle}{dt} = \frac{-i}{\hbar} \langle [A,H] \rangle \,. \tag{5}$$

So the fact [H, A] = 0 implies the quantity  $\langle A \rangle$  is conserved in a system evolving according to a choice of H. Conversely,  $\langle H \rangle$  is conserved in a system evolving with Hamiltonian A. So we say the symmetry is encoded in our commutator bracket. One should note this expression relates expectation values and is thus independent of the choice of Schrödinger or Heisenberg picture. Later we will see the phase space formulation shares the same consequence.

## **III. QUANTIZATION**

Now we will look more closely at this correspondence by introducing the concept of a quantization. A quantization is formally a map  $\Phi$  sending a smooth function in our phase space to an operator on a Hilbert space. We attribute to Dirac a number of axioms we expect such a map to uphold. [2] First, based on the analogues observed above, we expect the commutator to be compatible with the Poisson bracket for any two smooth functions A and B i.e.

$$[\Phi[A], \Phi[B]] = i\hbar\Phi[\{A, B\}] \tag{6}$$

Thus we see classical symmetries are preserved between Poisson and commutator algebras. Next we require constant functions correspond to a multiple of the identity, 1, explicitly

$$\Phi[1] = i\hbar \mathbf{1}.\tag{7}$$

Thus we recover the canonical commutation relation  $[\Phi[q], \Phi[p]] = i\hbar \mathbf{1}$  and retain associated relations such as the uncertainty principle. Finally, we expect a complete set of Poisson commuting functions to correspond to a complete set of commuting observables for a quantum system, a rather intricate relation.

Even substituting the latter for the simpler requirement that  $\Phi[q] = q$  and  $\Phi[P] = \partial_q$ , there is a theorem of Groenewold that such a perfect quantization does not exist. [3] Instead, attempts to map between classical and quantum observables must drop a requirement. One such example is the construction of geometric quantization

$$\Phi[f] = -i\hbar\nabla_{v_f} + f$$

where  $\cdot$  is simply multiplication and  $\nabla_{v_f}$  is an innocent notation for a covariant derivative locally along the Hamiltonian vector field from Equation 4. For each component, there is a gauge term added to the derivative obeying a particular quantization condition. On many manifolds, the first two properties hold which is desired for highly theoretical applications such as Chern-Simons Topological Quantum Field Theories. [4] For our purposes, we will instead relax the Poisson bracket - commutator compatibility in what is known as a deformation quantization. This will allow us to treat familiar systems such as the harmonic oscillator without complex topological restrictions.

Constructing a quantization may seem obvious at first glance - we are used to the canonical or Schrodinger quantization, for example by sending q to multiplication by itself and p to a derivative. This works fine for common systems until one encounters an expression such as qp, which is not excluded as a conserved quantity in arbitrary coordinates. Now we must decide on the order to apply our operators. Such an unambiguous ordering may also appear obvious such as to first apply every p, the Wick ordering, or to take the average of all ordered permutations, the Weyl ordering. However, as Groenewold's proof shows, any ordering breaks the Poisson bracket commutator compatibility relation for terms of degree four or larger. The reader may wish to verify that under the Weyl ordering, the following counterexample holds:

$$\{q^3, p^3\} = \{q^2 p, qp^2\} \left[\Phi[q^3], \Phi[p^3]\right] \neq \left[\Phi[q^2 p], \Phi[qp^2]\right].$$

Losing this relation may seem a tragic loss, however we will develop a formalism so that the error is of order  $\hbar^3$ . As a result, in the classical limit as  $\hbar \to 0$ , we will recover Hamiltonian dynamics.

## IV. PHASE SPACE OPERATOR ALGEBRA

Beginning from the symmetric Weyl ordering of polynomials, we seek a more general map from smooth functions on a manifold to operators on a Hilbert space. Fixing two operators Q and P on a Hilbert space obeying the canonical commutation relation (such as the standard Schrödinger operators on the space of normalizable functions of position), one such choice is the Weyl map, which for one coordinate may be written as

$$\Phi[A] = \iiint_{-\infty}^{\infty} \frac{dp dq da db}{(2\pi)} A(q, p) e^{ia(Q-q) + ib(P-p)}.$$
 (8)

At first glance, we notice this is simply a combination of a Fourier transform followed by an inverse Fourier transform into the operators Q and P rather than the original coordinates. One must be especially careful in noting that this object is an operator and thus the order of inverse transforms in Q and P does matter.

Now, making use of the non-commutative structure brought by applying the Baker-Campbell-Hausdorff formula, we note that powers of linear combinations of q, p correspond to powers of linear combinations of Q, P. From this, one may easily recovers the Weyl ordering for polynomials. Alternatively, we may instead invoke the fact the  $\exp(ibp)$  term generates translations in q in order to express every matrix element in the position basis (eigenstates of our particular Q)

$$\langle x | \Phi[A] | y \rangle = \int_{-\infty}^{\infty} \frac{dp}{(2\pi\hbar)} A\left(\frac{x+y}{2}, p\right) e^{ip(x-y)/\hbar}.$$
 (9)

This is convenient as we may then calculate expectation values without knowing the particular form the Q and P operators. [5]

Analogous to the Fourier transform (and in fact on the same function spaces as the Fourier transform), the Weyl quantization admits an inverse map from operators to functions known as the Wigner transform.

$$A(q,p) = 2 \int_{-\infty}^{\infty} dx \left\langle q + x \right| \Phi[A] \left| q - x \right\rangle e^{-i2px/\hbar}.$$
 (10)

We will soon see that this expression also provides a representation of the state of the system as a function on the original phase space.

While exploring analogies between the Fourier and Weyl transformations, we recall the existence of convolution. That is, by denoting the Fourier transform by a hat, that for two normalizable functions f and g, we can define another function f \* g such that  $\hat{f}(p)\hat{g}(p) = \widehat{f * g}(p)$ . For the Weyl transform, we can just as well require the existence of a so-called Moyal product A \* B such that for any smooth functions on our manifold A and B, we have

$$\Phi[A]\Phi[B] = \Phi[A \star B]. \tag{11}$$

We will now attempt to derive the resulting product from our Weyl quantization map. Ultimately, applying the inverse transform, Equation 10, to the product of the transforms, Equation 9, we combine terms using the Baker-Campbell-Hausdorff formula and eventually obtain a series expansion for  $A \star B$ . Following and simplifying Moyal's original procedure [6], we dispense with mathematical decorum and define a new left derivative operator  $\partial_q$  in contrast to the standard right derivative,  $\overrightarrow{\partial_q}$ . Here, the arrow represents the direction the operator acts, thus  $A\overrightarrow{\partial_q}B = \frac{\partial A}{\partial q}B$  while  $A\overrightarrow{\partial_q}B = A\frac{\partial B}{\partial q}$ . Then we can express the solution as a formal power series in these new derivatives as

$$A \star B = A \exp\left[i\hbar \left(\overleftarrow{\partial_q}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_q}\right)/2\right]B.$$
(12)

Though this expression seems rather unenlightened, it can in principle be calculated for any smooth function. Once the Moyal product is defined, we can finally probe the question of how the Wigner-Weyl quantization fails to preserve the commutator-Poisson bracket relation. Using linearity and equation 11 above, we have  $\Phi[A]\Phi[B] - \Phi[B]\Phi[A] = \Phi[A \star B - B \star A]$ . Thus we can now define the Moyal bracket of two functions, again expanding sine into complex exponentials then into a formal power series, as

$$\{\{A, B\}\} = (A \star B - B \star A) / (i\hbar)$$
$$= \frac{2}{\hbar} A \sin\left[\frac{\hbar}{2} \left(\overleftarrow{\partial_q} \overrightarrow{\partial_p} - \overleftarrow{\partial_p} \overrightarrow{\partial_q}\right)\right] B$$
(13)

Thus we immediately have the relation

$$[\Phi[A], \Phi[B]] = i\hbar\Phi[\{\{A, B\}\}],$$
(14)

indicating that our quantization has replaced our commutator not with the Poisson bracket but with the Moyal bracket. Conveniently, to zeroth order in  $\hbar$ , they correspond. Thus we expect behavior in our system beyond classical Hamiltonian behavior. This, we will see, manifests itself as decoherence.

## V. DENSITY MATRIX

To motivate our treatment of states in the phase space formulation, we will return to its original context - statistical mechanics. Recall that the ensemble average of a quantity A with particular fractions  $w_i$  being in eigenstate  $|a_i\rangle$  such that  $\Phi[A] |a_i\rangle = a_i |a_i\rangle$ , would simply be the weighted sum of the eigenvalues. Extrapolating to a more general basis  $b_i$ , we then have, by resolution of the identity,

$$\langle A \rangle = \sum_{i} w_i \langle a_i | A | a_i \rangle = \sum_{i,j} w_i \langle a_i | A | b_j \rangle \langle b_j | a_i \rangle.$$
(15)

Rearranging, we have

$$\langle A \rangle = \sum_{j} \langle b_{j} | \sum_{i} (w_{i} | a_{i} \rangle \langle a_{i} | A) | b_{j} \rangle = Tr[\rho A] \quad (16)$$

where we have defined the density matrix operator

$$\rho = \sum_{i} w_i \left| a_i \right\rangle \left\langle a_i \right|, \qquad (17)$$

where the sum is taken over a number of distinct states in an ensemble  $a_i$ . The corresponding density matrix we refer to is simply the operator expressed in in a given basis which is inherently Hermitian. This quantum density matrix corresponds to the semi-classical density  $\rho$  such that the ensemble average of a quantity in phase space is given by

$$\langle A \rangle = \int \rho(q, p) A(q, p) \left(\frac{dqdp}{2\pi\hbar}\right)^N$$
 (18)

. For the canonical ensemble, it is given by the expression  $\rho = \exp(-\beta H(q,p)) / \int \exp(-\beta H(q,p)) [dqdp/(2\pi\hbar)]^N$ . Clearly, this smooth function on phase space is positive everywhere. Given the correspondence above, we will indeed be able to associate a density with analogous expectation values. However, we will find discrepancies including negative values and dependence on  $\hbar$  in our classical density.[7]

## VI. WIGNER FUNCTIONS

Now that we've constructed the density matrix, a perfectly functional Hermitian operator, it is now reasonable to ask what the corresponding function through the Wigner transform could represent.

For our purposes, we will assume our system is one dimensional and in the pure state  $\langle x|\psi\rangle = \psi(x)$  but the following procedure is defined in general. Now applying the Wigner transform, Equation 10, to the density matrix operator, we arrive at the so-called Wigner Function,

$$W(q,p) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} \psi^*(q+x)\psi(q-x)e^{-i2px/\hbar}dx, \quad (19)$$

which we will see contains exactly the same information as the wavefunction.

Motivated by the analogous classical behavior in equation 18, we may define the expectation value of any observable A for a system with Wigner function W as the weighted integral in phase space given by

$$\langle \Phi[A] \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dq dp W(q, p) A(q, p).$$
 (20)

To interpret this expression, we will consider our canonical cases, q and p. Letting A(q,p) = q, we may perform the p integral first to see that  $\int dpW(q,p)$  really is the probability density of observing a given value of position meanwhile, allowing A = p, we see  $\int dqW(q,p)$  is the probability density of observing a given momentum. In this sense, the Wigner function treats the phase space variables symmetrically in contrast to the Fourier transform relationship in the canonical/Schrodinger case. Recall this was our original motivation for the Weyl quantization.

Along with symmetry, a number of unintended properties emerge from this definition of the Wigner function. By normalizability, we know each term in Equation 19 has a magnitude of at most one yet we cannot ensure the entire function is positive. In fact, only specific minimum uncertainty states are guaranteed positive. Above we saw that when evaluating an expectation value, the Wigner function integrates in both q and p to a probability density which is positive for a given state. Otherwise, we are able to bound the regions where this property fails as a function of  $\hbar$  which disappears in the classical limit.

Similarly, we cannot prevent an  $\hbar$ -dependence from appearing in our Wigner function. Instead, we observe this function is inherently quantum - it may live in the space of smooth functions on our classical manifold yet it depends on a parameter introduced by our quantization procedure. A simple example is the harmonic oscillator below in equation 26.

Before working on an example, we will need to address the dynamics of our system in the phase space formulation. Requiring evolution of expectation values as in equation 5, or by directly combining the Schrödinger equation with the definition of the Wigner function, we arrive at evolution again governed by the Moyal bracket: [8]

$$\frac{dW}{dt} = -\{\{W, H\}\}$$
(21)

Thus the value of the Wigner function does not follow the Hamiltonian time evolution of a classical function in phase space but a more unintuitive perturbation.

Finally, given our definitions above, one can derive given a position-basis energy eigenstate  $\psi_n$  that the corresponding Wigner functions  $W_n$  obey the phase-space relation

$$H(q,p) \star W_n(q,p) = E_n W_n(q,p). \tag{22}$$

Again our problem-solving can be reduced to a relation in the phase space.

Ultimately, we are able to describe our quantum system using not an element of an ambient Hilbert space but instead a real function of both position and momentum coordinates in phase space. However, unlike the classical motion generated from the Poisson bracket with the Hamiltonian, the Wigner function evolves with a deformed term which is non-local and generates decoherence.

## VII. COHERENCE AND DECOHERENCE

Ultimately, the phase space formulation provides insight into the definition of coherence - whether states can be constructed to evolve according to rigid classical behavior or not. This is generally useful for example in understanding optics of coherent squeezed states. If not, we can instead characterize the degree of decoherence in a given system - under which conditions the system may be treated as decoupled and semi-classical.

We know coherent states are generally constructed from energy eigenstates of the 1D harmonic oscillator, so we will start there using our new approach. Note, without reference to the form of the solutions in a Hilbert space, we can still be able to describe motion. For simplicity, consider q, p coordinates with constants absorbed so that  $H(q, p) = \frac{1}{2} (q^2 + p^2)$  so we arrive at the symmetric form of equation 22,

$$\left[\frac{1}{2}\left(p-\frac{i\hbar}{2}\partial_q\right)^2 + \left(q+\frac{i\hbar}{2}\partial_p\right)^2\right]W_n = E_nW_n \quad (23)$$

Here, we have simplified the exponentials in equation 12, remembering the translation relation  $\exp(-i(-i\hbar\partial_q)a/\hbar)H(q,p) = H(q - a, p)$  and antisymmetric equivalent for  $\partial_p$  where the remaining directional partial derivatives operators may be considered constants as commuting. To find a constraint on our solution, we use either the symmetry that  $H\star W_n-W_n\star H=0$  or the fact the solution is purely real to find

$$i\hbar(q\partial_p - p\partial_q)W_n = 0 \tag{24}$$

This reduces to a requirement of radial symmetry, that is,  $W_n(q, p) = W(q^2 + p^2)$ . The phase-space eigenvalue equation can now be expressed in the variable  $s = q^2 + p^2$ as

$$(s - 2E_n)W - \hbar^2(W_s + sW_{ss}) = 0$$
(25)

with series solution around the singular point s = 0 converging only when  $E_n = \hbar\omega(n + 1/2)$  as expected. In this case, the solution may be expressed as the product of a Laguerre polynomial and Gaussian, as tedious of a calculation as the Hermite polynomials in the traditional solution:

$$W_n = \frac{(-1)^n}{\pi\hbar} L_n \left(\frac{q^2 + p^2}{\hbar/2}\right) e^{-(q^2 + p^2)/\hbar}.$$
 (26)

In principle, one could compute the evolution of any displaced linear combination of these harmonic oscillator states using numerical methods. However, for this simple potential, we know the classical trajectories are rigid rotation. Thus, classical quantities such as x and p and the associated expectations ought to rotate from their initial values. We see here, that though the Wigner functions are phase space densities, they depend on the quantity  $\hbar$ from quantization and are negative over large regions.

Ultimately, even our evolution for the Wigner function is Hamiltonian, that is, determined entirely by the Poisson bracket.

$$\begin{aligned} \frac{dW}{dt} &= \{\{H, W\}\} = q \frac{\partial W}{\partial p} - p \frac{\partial W}{\partial q} \\ &= \frac{\partial H}{\partial q} \frac{\partial W}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial W}{\partial q} \\ &= \{H, W\} \end{aligned}$$

In other words, the Wigner function also rigidly rotates periodically and without dispersion. For a general Hamiltonian, this will not be the case as additional terms will arise in the expansion of the Moyal bracket. [3]

One such example is a system placed in a heat bath which introduces a term into the Moyal bracket of the form  $D \frac{\partial^2 W}{\partial p^2}$ . Given a superposition of Gaussians with standard deviation  $\delta$  separated by a distance  $\ell$ , the Wigner function includes an oscillatory term of the form

$$W_{osc}(q,p) = \frac{1}{\pi\hbar} \exp\left(-\frac{p^2 \delta^2}{\hbar^2} - \frac{q^2}{\delta^2}\right) \cos\left(\frac{\ell p}{\hbar}\right) \quad (27)$$

Ultimately, this oscillation will decay away due to the extra term in the bracket, in a process known as decoherence. Thus, the system recovers the classical behavior of two independent wavepackets on a sufficiently large timescale. This characteristic loss of entangled information is perhaps only explicit from this perspective. [9] In more generality, decoherence is a very separate concept from coherence. Ultimately a more thorough analysis with density operators would reveal conditions in which terms in the Wigner function are suppressed. These then correspond to cases in which a block of the density matrix may be treated as an independent system. For example in the above system, the left and right wave packets become thoroughly decohered from each other.

### VIII. CONCLUDING REMARKS

Overall, we have demonstrated one specialized quantization procedure which allows us consider states as semiclassical densities on phase-space without looking into a Hilbert space, though we are free to consider the corresponding operators there. We do note that other invertible transforms constructed from different orderings are possible. For example, if instead of symmetrically applying the Q and P operators, we instead substituted and ordered harmonic oscillator creation and annihilation operators, we would have arrived at the popular Segal-Bargmann quantization. In any case, we could recalculate the Moyal star product and bracket by its defining property, equation 11. For many choices, the bracket will still be a deformation of the Poisson, that is, equal in the limit  $\hbar \to 0$ . [4] Ultimately, there are many formulations of quantum mechanics which provide consistent expectation values and have semiclassical interpretations - each providing insight into particular systems.

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