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## Phase space quantum mechanics - Direct

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Conventional approach to quantum mechanics in phase space,  $(q, p)$ , is to take the operator based quantum mechanics of Schrödinger, or an equivalent, and assign a  $c$ -number function in phase space to it. We propose to begin with a higher level of abstraction, in which the independence and the symmetric role of  $q$  and  $p$  is maintained throughout, and at once arrive at phase space state functions. Upon reduction to the  $q$ - or  $p$ -space the proposed formalism gives the conventional quantum mechanics, however, with a definite rule for ordering of factors of noncommuting observables. Further conceptual and practical merits of the formalism are demonstrated throughout the text. © 2006 American Institute of Physics.

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### I. INTRODUCTION

Wigner's 1932 initiative<sup>1</sup> is a reformulation of the operator based quantum theory of Schrödinger in the language of  $c$ -number distribution functions in a phase space. His prescription, however, turns out to have a feature extra to what one finds in Schrödinger's theory. There is nothing in the founding principles of the operator based theory to prescribe a rule for ordering of the factors of noncommuting operators in a product. In contrast, Wigner's formalism, upon reduction from phase space to the configuration space, acquires Weyl's ordering,<sup>2,3</sup> How and at what stage, in going from Schrödinger's state functions in configuration space to those of Wigner in phase space and again coming back to the configuration space, acquires Weyl's ordering creep in? This feature is not unique to Wigner's functions. Other distributions exist in the literature, e.g., Kirkwood,<sup>4</sup> Husimi,<sup>5</sup> Margenau and Hill,<sup>6</sup> Torres-Vega and Frederick,<sup>7-9</sup> Li *et al.*,<sup>10</sup> de Gosson,<sup>11,12</sup> etc. Each of them carries its own ordering rule, with no precedence in the configuration space formalism. Can one conjecture that the phase space formulations of quantum mechanics are more complete than their configuration space counterpart, because of their built-in ordering rules? If so, there should be a way to arrive at phase space formulations without reference to the conventional operator based theory. Here we argue that in the classical dynamics and classical statistical dynamics (Liouville's equation) the generalized coordinates and momenta,  $q$  and  $p$ , respectively, play symmetric and more importantly, independent roles. In the operator based quantum theory one or the other loses its identity at the expense of the other and the formalism reduces to one in either  $q$  or  $p$  space. One could avoid this by carrying the  $q$  and  $p$  formalisms concomitantly and at once arrive at state functions in  $qp$  spaces. The so-obtained state functions are the  $qp$  representa-

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tion of the mixed states of quantum statistical mechanics. The operator based theory emerges as a special case of this general one, but this time with a definite ordering rule for noncommutative operators. The rule depends on the nature of the  $q$  and  $p$  variables, adopted initially.

## II. EXTENSION OF THE CLASSICAL DYNAMICS

Let  $q = \{q_i(t), i = 1, \dots, N\}$  be the collection of the generalized coordinates describing the state of motion of a dynamical system. It is customary to assign a Lagrangian,  $L^q(q, \dot{q})$ , to the system, define the conjugate momenta,  $p = \partial L^q / \partial \dot{q}$ , and construct the  $H(q, p) = \dot{q}p - L^q$ . One may do this the other way around. Begin with a given  $H(q, p)$  and find  $L^q(q, \dot{q})$  as a solution of the following differential equation;

$$H\left(q, \frac{\partial L^q}{\partial \dot{q}}\right) - \dot{q} \frac{\partial L^q}{\partial \dot{q}} + L^q = 0. \quad (1)$$

One may, however, carry out the same procedure with  $q$  replaced by  $p$  and arrive at a  $L^p(p, \dot{p})$  satisfying the differential equation

$$H\left(\frac{\partial L^p}{\partial \dot{p}}, p\right) + \dot{p} \frac{\partial L^p}{\partial \dot{p}} - L^p = 0. \quad (2)$$

The use of  $L^p$  to study the evolution of a dynamical system is not a common practice. But it is a possibility and has precedence.<sup>13</sup> There is no bar to employing the two alternatives simultaneously. We follow Sobouti and Nasiri<sup>14</sup> (hereafter, paper I) and define the “extended Lagrangian”

$$\mathcal{L}(q, \dot{q}; p, \dot{p}) = -\dot{q}p - q\dot{p} + L^q(q, \dot{q}) + L^p(p, \dot{p}). \quad (3)$$

The first two terms on the right-hand side constitute a total time derivative and are introduced for later convenience. One may now write down the Euler-Lagrange equations for  $q$  and  $p$ ,

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = \frac{d}{dt} \frac{\partial L^q}{\partial \dot{q}} - \frac{\partial L^q}{\partial q} = 0, \quad (4a)$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{p}} - \frac{\partial \mathcal{L}}{\partial p} = \frac{d}{dt} \frac{\partial L^p}{\partial \dot{p}} - \frac{\partial L^p}{\partial p} = 0. \quad (4b)$$

Equation (4a) is the conventional equation of motion in  $q$  space. With preassigned initial values  $q(t_0)$  and  $\dot{q}(t_0)$  at  $t_0$  it can be solved for the orbits  $q(t)$  in  $q$  space. Similarly, with given initial values  $p(t_0)$  and  $\dot{p}(t_0)$ , Eq. (4b) can be solved for the orbits  $p(t)$  in the  $p$  space. The conditions for  $q$  and  $p$  orbits to represent the same state of motion of the system are  $p(t_0) = \partial L^q / \partial \dot{q}|_{t_0}$  and  $q(t_0) = \partial L^p / \partial \dot{p}|_{t_0}$ . Such a state of motion will be referred to as a “pure state.” Otherwise it will be called a “mixed state” of motion. The nomenclature is from the statistical quantum mechanics and it will be seen later that they imply the same notions as therein. On a pure state  $p$  and  $q$  are initially canonically conjugate pairs and it is shown in paper I that once they are canonically conjugate at one time they remain so for all times. On the other hand there are no restrictions on the initial values of  $q$  and  $p$  on mixed states. Therefore,  $q(t)$  and  $p(t)$  remain unrelated and evolve independently. The existence of the extended Lagrangian  $\mathcal{L}(q, \dot{q}; p, \dot{p})$ , however, permits the following “extended momenta” to be defined:

$$\pi_q = \frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial L^q}{\partial \dot{q}} - p, \quad (5a)$$

$$\pi_p = \frac{\partial \mathcal{L}}{\partial \dot{p}} = \frac{\partial L^p}{\partial \dot{p}} - q. \quad (5b)$$

These in turn allow an “extended Hamiltonian” to be defined through the following Legendre transformation;

$$\mathcal{H}(q, \pi_q; p, \pi_p) = \dot{q} \pi_q + \dot{p} \pi_p - \mathcal{L}(q, \dot{q}; p, \dot{p}). \quad (6)$$

To eliminate  $\dot{q}$  and  $\dot{p}$  from  $\mathcal{H}$  one substitutes (a) for  $\mathcal{L}$  from Eq. (3), (b) for  $L^q$  and  $L^p$  from Eqs. (1) and (2), and (c) for  $\partial L^q / \partial \dot{q}$  and  $\partial L^p / \partial \dot{p}$  from Eqs. (5a) and (5b). One arrives at

$$\mathcal{H}(q, \pi_q; p, \pi_p) = H(q, p + \pi_q) - H(q + \pi_p, p) = \sum_{n=0} \frac{1}{n!} \left[ \frac{\partial^n H}{\partial p^n} \pi_q^n - \frac{\partial^n H}{\partial q^n} \pi_p^n \right], \quad (7)$$

where the derivatives are to be evaluated at  $(q, p)$ . We leave it to the reader to familiarize him/herself with  $\mathcal{H}$  by writing down four Hamilton’s equations for  $\dot{q}$ ,  $\dot{\pi}_q$ ,  $\dot{p}$ , and  $\dot{\pi}_p$ . Here, the condition for pure state motions is  $\pi_q(t_0) = \pi_p(t_0) = 0$ , and once they are initially zero they remain so for all times. Then by Eqs. (5a) and (5b)  $q$  and  $p$  turn into canonically conjugate pairs for all times (paper I). To summarize, for any dynamical system we introduce an extended phase space,  $(q, \pi_q; p, \pi_p)$ , extended momenta, Lagrangians, and Hamiltonians. All concepts and procedures of the conventional dynamics are extendible to this extended dynamics. Of particular relevance to this paper, which will be referred to shortly, are: (1) canonical transformations from one set of variables  $(q, \pi_q; p, \pi_p)$  to another, and (2) Poisson’s brackets extended as

$$\{F, G\} = \frac{\partial F}{\partial q} \frac{\partial G}{\partial \pi_q} - \frac{\partial F}{\partial \pi_q} \frac{\partial G}{\partial q} + \frac{\partial F}{\partial p} \frac{\partial G}{\partial \pi_p} - \frac{\partial F}{\partial \pi_p} \frac{\partial G}{\partial p}. \quad (8)$$

### III. QUANTUM DYNAMICS IN $qp$ SPACE

Now that we have the extended the Hamiltonian of Eq. (7) we may construct a quantum mechanics in  $qp$  space. We do this on the following premises.

(1) Let  $\mathcal{X}$  be the function space of all integrable complex functions  $\chi(q, p)$ . Let  $q, \pi_q, p$ , and,  $\pi_p$  be operators on  $\mathcal{X}$ , satisfying the commutation rules

$$[q, \pi_q] = [p, \pi_p] = i \hbar, \quad [q, p] = [\pi_q, \pi_p] = [q, \pi_p] = [p, \pi_q] = 0. \quad (9)$$

These are the fundamental Poisson brackets of Eq. (8), promoted to commutation brackets by Dirac’s prescription. Note the manifest independence of  $q$  and  $p$  in the vanishing of their commutation brackets.

(2) By virtue of Eq. (9),  $\mathcal{H}$  is now an operator on  $\mathcal{X}$ . Let  $\chi(q, p, t) \in \mathcal{X}$  be a state function satisfying the Schrödinger-type equation

$$i \hbar \frac{\partial \chi}{\partial t} = \mathcal{H} \chi = \left[ H \left( q, p - i \hbar \frac{\partial}{\partial q} \right) - H \left( q - i \hbar \frac{\partial}{\partial p}, p \right) \right] \chi. \quad (10)$$

(3) Let the rule to evaluate the expectation values of an observable  $O(q, p)$ , a real c-number operator on  $\mathcal{X}$ , be

$$\langle O(q, p) \rangle = \int O(q, p) \text{Re } \chi dq dp = \frac{1}{2} \int O(q, p) (\chi + \chi^*) dq dp. \quad (11)$$

We will return to this averaging rule shortly, and revise it. The logic behind it, however, is to be noted, the averages of observables should be real. In what follows we demonstrate that (1) the formalism so designed is a theory of quantum ensembles in phase space. Its pure state case is the conventional quantum mechanics, however, with a definite ordering rule accompanying it. (2) It

can be transformed to other phase space formalisms, including to that of Wigner, by suitable unitary or similarity transformations on  $\mathcal{X}$ . The latter in turn originates from suitable canonical transformations from one extended phase space coordinate to another.

### A. Solutions of Eq. (10)

To begin with,  $\chi$  is of the form

$$\chi(q,p) = F(q,p)e^{-ipq/\hbar}. \quad (12)$$

The exponential factor is a consequence of the total time derivative,  $-d(qp)/dt$  in Eq. (3). It is easily verified that

$$\left(p - i\hbar \frac{\partial}{\partial q}\right)\chi = i\hbar \frac{\partial F}{\partial q} e^{-ipq/\hbar}, \quad (13a)$$

$$\left(q - i\hbar \frac{\partial}{\partial p}\right)\chi = i\hbar \frac{\partial F}{\partial p} e^{-ipq/\hbar}. \quad (13b)$$

Substitution of Eqs. (13) and (12) in Eq. (10) gives

$$i\hbar \frac{\partial F}{\partial t} = \left[ H\left(q, -i\hbar \frac{\partial}{\partial q}\right) - H\left(-i\hbar \frac{\partial}{\partial p}, p\right) \right] F. \quad (14)$$

The operators on the right-hand side of Eq. (14) are recognized as the Hamiltonians of the conventional quantum mechanics, the first in  $q$  and the second in  $p$  representation. Thus, one obtains the superposition of the separable solutions

$$\chi(q,p,t) = \sum_{\alpha,\beta} A_{\alpha\beta} \psi_{\alpha}(q,t) \phi_{\beta}^*(p,t) e^{-ipq/\hbar}, \quad (15)$$

where

$$i\hbar \frac{\partial \psi_{\alpha}}{\partial t} = H\left(q, -i\hbar \frac{\partial}{\partial q}\right) \psi_{\alpha}, \quad (16a)$$

$$i\hbar \frac{\partial \phi_{\beta}}{\partial t} = H\left(i\hbar \frac{\partial}{\partial p}, p\right) \phi_{\beta}. \quad (16b)$$

To each  $\psi_{\alpha}(q)$  there corresponds a  $\phi_{\alpha}(p)$  that are Fourier transforms of each other,

$$\psi_{\alpha}(q) = \frac{1}{(2\pi\hbar)^{N/2}} \int \phi_{\alpha}(p) e^{ipq/\hbar} dp, \quad (17)$$

where  $N$  is the number of degrees of freedom of the system.

### B. The averaging rule revisited: Acceptable state functions

Let  $Q(q)$  be an observable represented by a real polynomial or series in  $q$ . Its matrix representation,  $\hat{Q}$ , in either  $\chi$ -,  $\psi$ -, or  $\phi$ -basis is Hermitian. Thus

$$\begin{aligned} Q_{\beta\alpha} &= \int \psi_\alpha(q) Q(q) \psi_\beta^*(p) e^{-ipq/\hbar} dp dq \\ &= \int \psi_\beta^*(q) Q(q) \psi_\alpha(q) dq = \int \phi_\beta^*(p) Q\left(i\hbar \frac{\partial}{\partial p}\right) \phi_\alpha(p) dp = Q_{\alpha\beta}^*, \end{aligned} \quad (18)$$

where we have used the fact that  $\psi$  and  $\phi$  bases are the Fourier transforms of each other. The coefficient  $(2\pi\hbar)^{-N/2}$  is suppressed for brevity. The expectation value of  $Q$ , by Eq. (11), now becomes

$$\langle Q \rangle = \frac{1}{2} \int Q(\chi + \chi^*) dp dq = \frac{1}{2} \text{tr}[\hat{Q}(\hat{A} + \hat{A}^\dagger)], \quad (19)$$

where  $\hat{A}$  is the matrix of  $A_{\alpha\beta}$  of Eq. (15). This gives the freedom of choosing  $\hat{A} = \hat{A}^\dagger$  and of simplifying Eq. (11) to read  $\langle Q \rangle = \int Q \chi dp dq = \text{tr}(\hat{Q}\hat{A})$ . Choosing  $Q(q) = 1$ , imposes the further restriction  $\text{tr}\hat{A} = 1$ . Requiring the averages of all positive definite functions of  $q$  to be positive still restricts  $\hat{A}$  to be a positive definite matrix. Had one chosen a differentiable function  $P(p)$  instead of  $Q(q)$ , one still would have arrived at the same requirements for  $\hat{A}$ . To summarize,  $\chi$  of Eq. (15) is a physically acceptable solution if

$$\hat{A} = \hat{A}^\dagger, \text{ positive definite, and } \text{tr}\hat{A} = 1. \quad (20)$$

With this provision the averaging rule of Eq. (11) for  $Q(q) + P(p)$  reduces to

$$\langle Q(q) + P(p) \rangle = \int (Q + P) \chi dp dq. \quad (21)$$

For a product  $Q(q)P(p)$ , by the prescription of Eq. (11) and with the restrictions of Eq. (20) on  $\hat{A}$ , one has

$$\langle QP \rangle = \text{Re} \text{tr}(\hat{Q}\hat{P}\hat{A}) = \frac{1}{2} \text{tr}(\hat{Q}\hat{P}\hat{A} + \hat{A}\hat{P}\hat{Q}) = \text{tr}\left[\frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})\hat{A}\right], \quad (22)$$

where  $\hat{Q}$  and  $\hat{P}$  are the matrix representations of  $Q(q)$  and  $P(p)$  as in Eq. (18). Translation of this to the  $q$  space language, say, is

$$\langle QP \rangle = \frac{1}{2} A_{\alpha\beta} \int \psi_\beta^*(q) \left[ Q(q) P\left(-i\hbar \frac{\partial}{\partial q}\right) + P\left(-i\hbar \frac{\partial}{\partial q}\right) Q(q) \right] \psi_\alpha dq. \quad (23)$$

Thus, upon reduction of the formalism of the present paper to that of the  $q$ -space, the ordering rule associated with a product  $Q(q)P(p)$  is the symmetric ordering. It has emerged from the formalism itself, unlike the ad hoc ordering rules of the conventional quantum mechanics.

### IV. MORE ABOUT EQ. (10)

It was stated earlier that the proposed dynamics is essentially that of the ensembles. Here we elaborate on this, and show that (1) the classical limit of the theory is Liouville's equation that governs the dynamics of classical ensembles. (2) Its pure state case is Schrödinger's operator based theory. (3) In its full generality the theory gives von Neumann's density matrix and the evolution equation associated with it.

### A. Classical correspondence

In Eq. (10) expanding the Hamiltonian operators about  $(q, p)$ , and retaining only the first terms in the expansion, gives

$$\frac{\partial \chi}{\partial t} + \frac{\partial H}{\partial p} \frac{\partial \chi}{\partial q} - \frac{\partial H}{\partial p} \frac{\partial \chi}{\partial p} = \frac{d\chi}{dt} = 0. \quad (24)$$

This is the Liouville equation for the distribution function of classical ensembles. Its most general solutions are  $\chi[q(t), p(t)]$ , where  $q(t)$  and  $p(t)$  are the classical trajectories in  $q$  and  $p$  spaces. The two trajectories may represent the same state of motion if they satisfy the conditions of initial canonical conjugacy narrated below Eq. (4). Otherwise, they remain independent and evolve independently. It is this classical notion of independence that we have carried through to the quantum formalism. Let us also note that the reduction of the phase space evolution equation to the classical Liouville's equation is a common feature of all such formalisms.

### B. Schrödinger's case

Allowance for only one term in Eq. (15) reproduces the conventional quantum mechanics in all its details. Thus

$$\chi = \psi(q) \phi^*(p) e^{-ipq/\hbar}, \quad (25a)$$

$$i \hbar \frac{\partial \psi}{\partial t} = H\left(q, -i \hbar \frac{\partial}{\partial q}\right) \psi, \quad (25b)$$

$$\psi \text{ and } \phi \text{ Fourier transforms of each other,} \quad (25c)$$

$$\int \chi dp dq = \int \psi^* \psi dq = \int \phi^* \phi dp = 1, \quad (25d)$$

$$\langle Q(q)P(p) \rangle = \frac{1}{2} \int \psi^* \left[ p \left( -i \hbar \frac{\partial}{\partial q} \right) Q(q) + Q(q) P \left( -i \hbar \frac{\partial}{\partial q} \right) \right] \psi dq. \quad (25e)$$

Heisenberg's uncertainty principle follows immediately from Eq. (25) that one may find in standard texts in quantum mechanics. The ordering rule of Eq. (25e) is, however, the added feature of the theory.

### C. Density matrix and von Neumann's equation

The state function of Eq. (15), as it stands represents the state of an ensemble in a mixed state. If the matrix  $\hat{A}$  is diagonalized to  $A_{\alpha\beta} = A_{\alpha} \delta_{\alpha\beta}$ ,  $\chi$  reduces to  $\chi = \sum A_{\alpha} \psi_{\alpha} \phi_{\alpha}^* e^{-ipq/\hbar}$ . Upon integration over  $q$  or  $p$  one immediately recognizes  $A_{\alpha}$  as the probability of the system to be in the state  $\psi_{\alpha}(q, t)$  or  $\phi_{\alpha}(p, t)$ . One may, however, do better. Let  $\{\phi_n(q)\}$  be a complete orthonormal time independent basis set, and  $\{\phi_n(p)\}$  be its Fourier replica. These basis sets are not required to be the eigenstates of  $H(q, p)$ , though this is a possibility. Hereafter, to avoid the ambiguity, we use the Latin subscripts to denote the members of the basis set and reserve Greek subscripts to denote the solutions of Eqs. (16a) and (16b). Expansion of  $\chi$  in these bases assumes the form  $\chi(q, p, t) = A_{mn}(t) \psi_n(q) \phi_m^*(p) e^{-ipq/\hbar}$ . Substituting this form in Eq. (10), multiplying the resulting equation by  $\psi_n^*(q) \phi_m(p) e^{ipq/\hbar}$ , and integrating over  $q$  and  $p$  gives

$$i\hbar \frac{d\hat{A}}{dt} = [\hat{A}, \hat{H}], \quad \hat{A} = \hat{A}^\dagger \quad \text{positive definite and } \text{tr} \hat{A} = 1, \quad (26)$$

where  $\hat{A}$  is the matrix of the expansion coefficients and  $\hat{H}$  that of the  $H(q, p)$  in either  $\chi$ -,  $\psi$ -, or  $\phi$ -basis. Equation (26) is von Neumann's equation for the evolution of the density matrix. As is known the case  $\text{tr}(\hat{A}^2) = \text{tr} \hat{A} = 1$  represents an ensemble in a pure state. If  $\text{tr}(\hat{A}^2) < 1$ , the ensemble is in a mixed state.

## V. CANONICAL TRANSFORMATIONS

All machinery of the canonical transformations from one extended coordinate system to another and their associated unitary or similarity transformations in the function space are available for a forage of deliberations. Except for a passing remark on the prospects of fuller uses of this approach at the end of this section, here we confine ourselves to one one-parameter family of transformations of which Wigner's state function emerges as a special case. Husimi's all positive distribution functions are also briefly mentioned.

Consider the infinitesimal transformations

$$q = Q - \delta\alpha\Pi_p, \quad \pi_q = \Pi_Q; \quad p = P - \delta\alpha\Pi_Q, \quad \pi_p = \Pi_P, \quad (27)$$

The generator of the transformation is  $G = \pi_p \pi_q$ . To this (and for a finite  $\alpha$ ) there corresponds the unitary operator

$$U_\alpha = e^{-i\alpha G/\hbar} = e^{i\hbar\alpha\partial^2/\partial q\partial p}, \quad U_\alpha^\dagger U_\alpha = 1, \quad (28)$$

in the function space. Operating by  $U_\alpha$  on a pure state function  $\chi(q, p, t) = \psi(q)\phi^*(p) \times \exp(-ipq/\hbar)$  generates another state function (let us call it  $\alpha$ -representation)

$$\chi(q, p, t) = U_\alpha \chi = \left(\frac{1}{2\pi\hbar}\right)^N \int \psi(q - \alpha\tau)\psi^*(q + (1 - \alpha)\tau)e^{ip\tau/\hbar} d\tau. \quad (29)$$

See the Appendix for proof of Eq. (29). For  $\alpha = 1/2$ , Eq. (29) gives Wigner's standard function,<sup>15,16</sup>  $\chi_{1/2} = W(q, p, t)$ . The cases  $\alpha = 0$  and 1 simply give back  $\chi$  and  $\chi^*$  of this paper, respectively. Similarly, operation by  $U_\alpha$  on Eq. (10) gives the evolution equation for  $\chi_\alpha$ ,

$$i\hbar \frac{\partial \chi_\alpha(q, p, t)}{\partial t} = i\hbar \frac{\partial}{\partial t} (U_\alpha \chi) = (U_\alpha \mathcal{H} U_\alpha^\dagger) U_\alpha \chi, \quad (30)$$

$$i\hbar \frac{\partial \chi_\alpha(q, p, t)}{\partial t} = \mathcal{H}_\alpha \chi_\alpha = -\frac{\hbar^2(1 - 2\alpha)}{2m} \frac{\partial^2}{\partial q^2} \chi_\alpha - i\hbar \frac{p}{m} \frac{\partial}{\partial q} \chi_\alpha$$

$$+ \sum_{n=0} \frac{(-\alpha)^n - (1 - \alpha)^n}{n!} (-i\hbar)^n \frac{\partial^n V}{\partial q^n} \frac{\partial^n}{\partial p^n} \chi_\alpha.$$

See the Appendix for proof of Eq. (30). For  $\alpha = 1/2$ , even  $n$  terms in Eq. (30) cancel out and one again recovers Wigner's evolution equation.<sup>3</sup> See Eq. (A7).

### A. Assigning $q$ -space operators to phase space functions: Ordering rule

The phase space state functions are devised to evaluate the expectation values of a  $c$ -number observable,  $F(q, p)$ , by integrations over the phase space. Upon reduction to the  $q$  space, say,  $f(q, p)$  turns into a differential operator in terms of  $q$  and  $\pi_q$ . The questions are: (1) how are different factors of noncommuting  $q$  and  $\pi_q$  ordered in a given  $\alpha$ -representation? (2) Averaging a given  $F(q, p)$  with different  $\chi_\alpha$ 's gives different values, how do such averages change from one



$\alpha$ -representation to another? Let  $\hat{F}_\alpha(q, \pi_q)$  be the  $q$  space operator corresponding to the  $c$ -number monomial  $q^n p^m$  in phase space when averaged by  $\chi_\alpha$ . The defining equation for  $\hat{F}_\alpha(q, \pi_q)$  is

$$\langle q^n p^m \rangle_\alpha = \int q^n p^m \chi_\alpha dp dq = \int \psi^*(q) \hat{F}_\alpha(q, \pi_q) \psi(q) dq. \quad (31)$$

For the combination of  $\alpha=0$  and 1 corresponding to  $(\chi + \chi^*)$  of Eq. (11) this is already worked out in Eq. (25e) and is the symmetric ordering

$$q^n p^m \rightarrow \frac{1}{2}(q^n \pi_q^m + \pi_q^m q^n). \quad (32)$$

For a general  $\alpha$ , it is given in Eq. (A10),

$$q^n p^m \rightarrow \sum_{r=0}^m \binom{m}{r} ((1-\alpha)\pi_q)^r q^n (\alpha\pi_q)^{m-r}. \quad (33)$$

For  $\alpha=1/2$  this reduces to Weyl's ordering,<sup>2,3</sup> which is known to go with Wigner's functions. To answer the second question we note the following:

$$\langle q^n p^m \rangle_{\alpha=0} = \int q^n p^m \chi dq dp = \int q^n p^m U_\alpha^\dagger \chi_\alpha dq dp = \int U_\alpha(q^n p^m) \chi_\alpha dq dp = \langle U_\alpha(q^n p^m) \rangle_\alpha, \quad (34)$$

where by Eq. (29) we have used  $\chi = U_\alpha^\dagger \chi_\alpha$ . The conclusion is that  $q^n p^m$  averaged by  $\chi$  is the same as  $U_\alpha(q^n p^m)$  averaged by  $\chi_\alpha$ . Upon adoption of

$$U_\alpha = \sum \frac{(-i\alpha\hbar)^k}{k!} \frac{\partial^k}{\partial q^k} \frac{\partial^k}{\partial p^k}$$

and operation by it on  $q^n p^m$  one finds

$$\begin{aligned} U_\alpha(q^n p^m) &= \sum_{k=0}^{\text{smaller of } n \text{ or } m} (-i\hbar\alpha)^k k! \binom{n}{k} \binom{m}{k} q^{n-k} p^{m-k} \\ &= q^n p^m + (-i\hbar\alpha)mnq^{n-1}p^{m-1} + \frac{1}{2}(-i\hbar\alpha)^2 n(n-1)m(m-1)q^{n-2}p^{m-2} + \dots \end{aligned} \quad (35)$$

## B. Assigning phase space functions to $q$ space operators

To a given operator  $\hat{F}(q, \pi_q)$ , a Taylor-expanded series in whatever order of powers of  $q$  and  $\pi_q$ , we associate the following  $c$ -number function:

$$F(q, p) = \sum_{n,m} F_{mn} \chi_{nm} = \langle q | \hat{F} | p \rangle e^{-ipq/\hbar}, \quad (36)$$

where  $F_{mn} = \langle n | \hat{F} | m \rangle$  is the matrix element of  $\hat{F}$  in the basis of the eigenstates of  $\hat{H}(q, \pi_q)$ . This is actually the inverse of the procedure that we used in Eq. (31) to associate an operator with a  $c$ -number function (let  $\alpha=0$  and replace  $q^n p^m$  by  $F(q, p)$  in Eq. (33) to see the analogy). The second equality in Eq. (36) expresses the same in the ket- and bra- notation of Dirac.

The corresponding function in  $\alpha$ -representation is simply

$$F_\alpha(q,p) = U_\alpha F(q,p) = \sum_{n,m} F_{mn} U_\alpha \chi_{nm} = \int \langle q - \alpha\tau | \hat{F} | q + 1(1-\alpha)\tau \rangle e^{ip\tau/\hbar} d\tau. \quad (37)$$

This is actually the generalization of Eq. (29) for a general operator  $\hat{F}(q, \pi_q)$ . The rule for the product  $\hat{F} = \hat{A}\hat{B}$  is worked out in Eq. (A13):

$$F(q,p) = \langle q | \hat{A}(q, \pi_q) \hat{B}(q, \pi_q) | p \rangle e^{-ipq/\hbar} = \sum_{n=0}^{\infty} \frac{(-i\hbar)^n}{n!} \frac{\partial^n A(q,p)}{\partial p^n} \frac{\partial^n B(q,p)}{\partial q^n}. \quad (38)$$

One may also work out the  $\alpha$ -representation of Eq. (38):

$$\begin{aligned} F_\alpha(q,p) &= U_\alpha F(q,p) = A_\alpha \left[ q + i\hbar \alpha \frac{\partial}{\partial p}, p - i\hbar \alpha(1-\alpha) \frac{\partial}{\partial q} \right] B_\alpha(q,p) \\ &= \sum_{n=0}^{\infty} \frac{(i\hbar)^n}{n!} \left[ \alpha \frac{\partial}{\partial q_A} \frac{\partial}{\partial p_B} - (1-\alpha) \frac{\partial}{\partial p_A} \frac{\partial}{\partial q_B} \right]^n A_\alpha(q,p) B_\alpha(q,p). \end{aligned} \quad (39)$$

See Eq. (A17) for details of the derivation. In Sec. VII, we analyze Bloch's problem as an illustration of the use of the developments of the last two subsections.

### C. A remark on general transformations

An economical way of treating canonical transformations is the symplectic formalism. Let  $\boldsymbol{\eta}$  be the column vector  $(q, \pi_q; p, \pi_p)$ . The equations of the classical dynamics assume the following form

$$\dot{\boldsymbol{\eta}} = \mathbf{J} \frac{\partial \mathcal{H}}{\partial \boldsymbol{\eta}}, \quad (40)$$

where  $\mathcal{H}(\boldsymbol{\eta})$  is the extended Hamiltonian of Eq. (7) and  $\mathbf{J}$  is the symplectic metric

$$\mathbf{J} = \begin{pmatrix} j & 0 \\ 0 & j \end{pmatrix}, \quad j = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (41)$$

An infinitesimal canonical transformation from  $\boldsymbol{\eta}$  to  $\boldsymbol{\eta} + \delta\boldsymbol{\eta}$  is of the form

$$\boldsymbol{\eta} + \delta\boldsymbol{\eta} = \boldsymbol{\eta} - \epsilon \frac{\partial G(\boldsymbol{\eta})}{\partial \boldsymbol{\eta}}, \quad (42)$$

where  $G$  is the generator of the transformation and  $\epsilon$  indicates its infinitesimal character. The matrix of the transformation is

$$M_{ij} = \delta_{ij} - \epsilon \frac{\partial^2 G}{\partial \eta_i \partial \eta_j}. \quad (43)$$

The condition for canonicity is

$$\mathbf{M}\mathbf{J}\mathbf{M}^\dagger = \mathbf{J} + O(\epsilon^2). \quad (44)$$

This imposes the condition on  $G$  to be either linear in  $\eta_j$  or quadratic and symmetric in  $\eta_i, \eta_j$  or both. For clarity, hereafter we confine our discussion to a system of one degree of freedom,  $N = 1$ . The most general form of  $G$  with the restriction just mentioned is

$$G(\boldsymbol{\eta}) = a_i \eta_i + \alpha_{ij} \eta_i \eta_j, \quad i, j = 1, 2, 3, 4 \text{ correspond to } q, \pi_q; p, \pi_p, \quad (45)$$

where the four parameters  $a_i$  initiate translations and the ten symmetric  $\alpha_{ij}$  cause rotations, boosts, squeezes, scale changes, etc. The ten transformations  $\alpha_{ij}$  constitute a symplectic group  $SP(4)$ , and

is locally isomorphic to the (3+2)-dimensional Lorentz group. This is the group that Kim and Noz<sup>17</sup> encounter in their study of four-dimensional phase space consisting of two oscillators representation of  $O(3+2)$ , and proves to be a useful mathematical tool in quantum optics. To each of the fourteen transformations of Eq. (45) there corresponds a unitary or similarity transformation in the function space. That of Eq. (27) it is unitary. An example of nonunitary operators is the following. To the canonical coordinate transformation

$$q = Q + \frac{i\epsilon}{2\hbar}\Pi_Q + \frac{1}{2}\Pi_P, \quad \pi_q = \Pi_Q, \quad (46)$$

$$p = P + \frac{i\hbar}{2\epsilon}\Pi_P + \frac{1}{2}\Pi_Q, \quad \pi_p = \Pi_P,$$

there corresponds the complex similarity operator

$$S_\epsilon = \exp\left[\left(\frac{\epsilon}{4}\frac{\partial^2}{\partial q^2} + \frac{\hbar^2}{4\epsilon}\frac{\partial^2}{\partial p^2}\right) + \frac{i\hbar}{2}\frac{\partial^2}{\partial q \partial p}\right], \quad (47)$$

where  $\epsilon$  is a finite parameter of the transformation. Husimi's<sup>5</sup> all positive distribution in terms of  $\chi$  is

$$\chi_{\text{Hus}}(q, p, \epsilon) = S_\epsilon \chi(q, p). \quad (48)$$

## VI. BLOCH'S EQUATION IN PHASE SPACE

In this section we intend to illustrate some usage of the formalism developed so far. In any discussion of statistical mechanics, the partition function,  $Z(\beta) = \text{tr } \hat{\Omega}$ ,  $\hat{\Omega}(q, \pi_q) = \exp(-\beta \hat{H})$ , plays a pivotal role. Its calculation, however, is often cumbersome. One practice is to translate  $\hat{\Omega}$  and the corresponding Bloch's differential equation<sup>18</sup> into a phase space language,<sup>3,16</sup> solve the equation for a c-number  $\Omega(q, p, \beta)$  and calculate  $Z(\beta) = \int \Omega(p, q, \beta) dq dp$ . The ease of doing the job depends on the choice of the c-number assigned to  $\hat{\Omega}$ . Our suggestion is that of Eq. (36) Bloch's equation for  $\hat{\Omega}$  is

$$\frac{\partial \hat{\Omega}}{\partial \beta} = -\hat{H}\hat{\Omega} = -\hat{\Omega}\hat{H}. \quad (49)$$

We apply the rule of Eq. (36) to Eq. (49). Noting that  $\hat{H}(q, \pi_q) \rightarrow H(q, p) = p^2/2m + V(q)$  and using the product rule of Eq. (38) gives

$$-\frac{\partial \Omega(q, p; \beta)}{\partial \beta} = \left\{ H(q, p) - \frac{ip\hbar}{m}\frac{\partial}{\partial q} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} \right\} \Omega(p, q). \quad (50)$$

This same result is obtained in Ref. 19, however, by a totally different approach and through much lengthier calculations using Moyal's characteristic technique. Equation (49) in Wigner's representation is obtained by replacing  $\hat{\Omega}$  with  $\Omega_W(q, p; \beta)$ ,  $\hat{H}$  with  $p^2/2m + V(q)$  and using Eq. (A17) with  $\alpha=1/2$  to find the expression corresponding to  $\hat{H}\hat{\Omega}$ . In agreement with Refs. 3 and 16 one finds

$$-\frac{\partial \Omega_W(q, p; \beta)}{\partial \beta} = \left\{ \frac{p^2}{2m} - \frac{\hbar^2}{8m}\frac{\partial^2}{\partial q^2} + \sum_{n=0}^{n=\infty} \frac{(i\hbar/2)^n}{n!} \frac{\partial^n}{\partial q^n} V(q) \frac{\partial^n}{\partial p^n} \right\} \Omega_W(q, p; \beta). \quad (51)$$

The contrast between the two, Eqs. (50) and (51), is striking. The former is a second-order differential equation in  $q$  and the exact quantum effects in it appear as  $\hbar$  and  $\hbar^2$  only, while the latter in addition to  $\partial^2/\partial q^2$  is an  $n$ th-order differential equation in  $p$  and has all powers of  $\hbar$  in it.

In the following we solve Eq. (50) and give the partition functions for the simple harmonic and linear potentials.

### A. Simple harmonic potential

For  $H(q,p)=1/2(p^2/m+m\omega^2q^2)$  the solution is of the form

$$\Omega = \exp \left[ -A(\beta)H(q,p) - iB(\beta)\frac{pq}{\hbar} - C(\beta) \right]. \quad (52)$$

Substituting this in Eq. (50) and letting the coefficients of different powers of  $q$  and  $p$  vanish, gives

$$\frac{dA}{d\beta} = 1 - \hbar^2 \omega^2 A^2, \quad (53a)$$

$$\frac{dB}{d\beta} = \hbar^2 \omega^2 A(1 - B), \quad (53b)$$

$$\frac{dC}{d\beta} = \frac{1}{2} \hbar^2 \omega^2 A. \quad (53c)$$

The condition  $\Omega(q,p,0)=1$  imposes the boundary conditions  $A(0)=B(0)=C(0)=0$ . With these provisions one finds

$$A(\beta) = \frac{1}{\hbar \omega} \tanh \beta \hbar \omega, \quad (54a)$$

$$B(\beta) = \tanh \beta \hbar \omega \tanh \frac{\beta \hbar \omega}{2}, \quad (54b)$$

$$C(\beta) = -\frac{1}{2} \ln \cosh \beta \hbar \omega. \quad (54c)$$

The partition function is

$$Z(\beta) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \Omega(q,p,\beta) dq dp = \left[ 2 \sinh \frac{\beta \hbar \omega}{2} \right]^{-1}. \quad (55)$$

The normalized density function is  $\chi(q,p,\beta)=\Omega(q,p,\beta)/2\pi\hbar Z(\beta)$ , with low and high temperature limits

$$\chi = \frac{\sqrt{2}}{\pi\hbar} \exp \left[ -H(q,p) - \frac{ipq}{\hbar} \right], \quad \beta \hbar \omega \gg 1,$$

$$\chi = \frac{\beta\omega}{2\pi} \exp[-\beta H(q,p)], \quad \beta \hbar \omega \ll 1, \quad (56)$$

in agreement with the quantum and classical limits, respectively.

### B. Linear potential

The case is of interest for quark model,<sup>20</sup> where a sea of semi-infinite matter creates a linear potential  $V(q)=kq$ ,  $0 \leq q < \infty$ , and  $k > 0$ . By the same procedure above one obtains

$$\Omega(q, p, \beta) = \exp \left[ -\beta H - \frac{i\beta^2 p \hbar k}{2m} + \frac{\beta^3 \hbar^2 k^2}{6m} \right], \quad (57)$$

$$Z(\beta) = \sqrt{\frac{2\pi m}{\beta^3 k^2}} \exp \left[ \frac{\beta^3 \hbar^2 k^2}{24m} \right]. \quad (58)$$

$$\chi(q, p; \beta) = \sqrt{\frac{\beta^3 k^2}{2\pi m}} \exp \left[ -\beta H - \frac{i\beta^2 p \hbar k}{2m} + \frac{\beta^3 \hbar^2 k^2}{8m} \right]. \quad (59)$$

The corresponding Wigner's function<sup>21</sup> can be obtained by letting  $U_{1/2}$  operate on Eq. (59).

## VII. CONCLUSION

We have developed a quantum mechanics in phase space by carrying the independent and symmetric roles of  $q$  and  $p$ , so eminent in the Hamiltonian formulation of the classical mechanics, to quantum domain. This is done through the extension of the phase space by introducing the momenta  $\pi_q$  and  $\pi_p$  conjugate to  $q$  and  $p$ , respectively, and the subsequent extensions of the Lagrangians, Hamiltonians, Poisson's brackets, etc. In its full generality, the theory describes the dynamics of the quantum ensembles. Its pure state case is reducible to the conventional quantum mechanics in  $q$ - or  $p$ -spaces, however, with a definite rule for ordering of the factors of noncommuting operators. The latter feature is a direct consequence of the independence of  $q$  and  $p$  that is maintained at all stages of the formalism. Simple rules for assigning an operator  $\hat{F}(q, \pi_q)$  in  $q$ -space to a function  $F(q, p)$  in phase space and vice versa are prescribed. Extended canonical transformations enable one to go from one extended phase space to another. Correspondingly the associated unitary or similarity transformations in the function space enable one to generate further state functions from a given one. This unifying feature of the theory makes the comparison of the various functions existing in the literature possible and transparent.

To demonstrate the simplicity and the power of the formalism certain examples are worked out. Treatment of Bloch's equation, partition functions for simple harmonic and linear potentials, and the mathematical lemmas of the Appendix serve this end. Nasiri and Safari<sup>22</sup> and Razavi<sup>23</sup> have found the presented formalism of considerable assistance in their study of dissipative quantum systems.

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## APPENDIX

*Evaluation of  $\chi_\alpha = U_\alpha \chi$ :* By three Fourier and inverse Fourier transformations we convert  $\chi = \psi(q) \phi^*(p) \exp(-ipq/\hbar)$  into the following forms;

$$\chi = \int \phi(p') \phi^*(p'') \exp \frac{iq(p' - p'')}{\hbar} \exp \frac{ip\tau}{\hbar} \exp \frac{-ip''}{\hbar} dp' dp'' d\tau. \quad (A1)$$

By this provision we have moved both  $q$  and  $p$  variables to the exponent. Next we expand  $U_\alpha$  of Eq. (28) in power series, operate by it on the  $q$  and  $p$  exponents, and arrive at

$$\sum_{k=0}^{k=\infty} \frac{(i\alpha \hbar)^k}{k!} \frac{\partial^k}{\partial p^k} \frac{\partial^k}{\partial q^k} \exp \frac{iq(p' - p'')}{\hbar} \exp \frac{ip\tau}{\hbar} = \exp \frac{-i\alpha\tau(p' - p'')}{\hbar} \exp \frac{iq(p' - p'')}{\hbar} \exp \frac{ip\tau}{\hbar}. \quad (A2)$$

Using Eqs. (A1) and (A2) in the expression  $\chi_\alpha = U_\alpha \chi$ , and inverting  $\phi$ 's back to  $\psi$ 's gives Eq. (29),

$$\chi_\alpha(p, q, t) = U_\alpha \chi = \left( \frac{1}{2\pi\hbar} \right)^N \int \psi(q - \alpha\tau) \psi^*(q + (1 - \alpha)\tau) e^{ip\tau/\hbar} d\tau. \quad (\text{A3})$$

As mentioned earlier, for  $\alpha=1/2$  one recovers Wigner's standard state functions.

*Evolution equation for  $\chi_\alpha$ :* To prove Eq. (30), it is sufficient to evaluate  $\mathcal{H}_\alpha = U_\alpha \mathcal{H} U_\alpha^\dagger$ , where  $\mathcal{H}$  is the extended Hamiltonian of Eq. (10). It is easy to show that  $Q = U_\alpha q U_\alpha^\dagger = q - \alpha\pi_p$  and  $P = U_\alpha p U_\alpha^\dagger = p - \alpha\pi_q$ , which is the essence of the transformations of Eq. (27). We also note that

$$U_\alpha q^n p^m U_\alpha^\dagger = (q - \alpha\pi_p)^n (p - \alpha\pi_q)^m = (p - \alpha\pi_q)^m (q - \alpha\pi_p)^n. \quad (\text{A4})$$

We leave it to the reader to verify Eq. (A4) for him/herself for some small  $n$  and  $m$ . It is needless to say that  $[Q, P]=0$ , because the transformation is unitary. With these provisions one finds

$$\mathcal{H}_\alpha = H[q - \alpha\pi_p, p + (1 - \alpha)\pi_q] - H[q - (1 - \alpha)\pi_p, p - \alpha\pi_q]. \quad (\text{A5})$$

Expansion of the Hamiltonian about  $(q, p)$  gives

$$\mathcal{H}_\alpha = -\frac{\hbar^2(1-2\alpha)}{2m} \frac{\partial^2}{\partial q^2} - i\hbar \frac{p}{m} \frac{\partial}{\partial q} + \sum_{n=0} \frac{(-\alpha)^n - (1-\alpha)^n}{n!} (-i\hbar)^n \frac{\partial^n V}{\partial q^n} \frac{\partial^n}{\partial p^n}. \quad (\text{A6})$$

The Wigner case is for  $\alpha=1/2$ ,

$$\mathcal{H}_W = -i\hbar \frac{p}{m} \frac{\partial}{\partial q} + \sum_{n=0} \frac{1}{(2n+1)!} \left( \frac{\hbar}{2i} \right)^{2n+1} \frac{\partial^{2n+1} V}{\partial q^{2n+1}} \frac{\partial^{2n+1}}{\partial p^{2n+1}}. \quad (\text{A7})$$

*Ordering rule in  $\alpha$ -representation, proof of Eq. (33):* With Eqs. (31) and (A3) we have

$$\langle q^n p^m \rangle_\alpha = \int_{-\infty}^{+\infty} q^n \psi(q - \alpha\tau) \psi^*(q + (1 - \alpha)\tau) p^m e^{ip\tau/\hbar} dq dp d\tau. \quad (\text{A8})$$

Writing  $p^m$  as  $(i\hbar)^m \partial^m / \partial \tau^m$ , integrating by parts  $m$  times with respect to  $\tau$  frees the integrand from the  $p^m$  factor. Then integration with respect to  $p$  gives  $\delta(\tau)$ . Thus

$$\langle q^n p^m \rangle_\alpha = \int_{-\infty}^{+\infty} q^n (-i\hbar)^m \frac{\partial^m}{\partial \tau^m} [\psi(q - \alpha\tau) \psi^*(q + (1 - \alpha)\tau)] \delta(\tau) dq d\tau. \quad (\text{A9})$$

Next we substitute  $\partial / \partial \tau$  by  $\partial / \partial q$  with appropriate adjustments and carry out integrations by parts over  $q$  wherever necessary to free  $\psi^*$  and arrive at

$$\langle q^n p^m \rangle_\alpha = \int_{-\infty}^{+\infty} \psi^*(q) \left[ \sum_{r=0}^m \binom{m}{r} ((1 - \alpha)\pi_q)^r q^n (\alpha\pi_q)^{m-r} \right] \psi(q) dq. \quad (\text{A10})$$

The expression in the integrand is the desired ordering of Eq. (33), corresponding to  $q^n p^m$  in  $\alpha$ -representation. For  $\alpha=1/2$  one recovers Weyl's ordering

$$q^n p^m \rightarrow \left( \frac{1}{2} \right)^m \sum_{r=0}^m \binom{m}{r} \pi_q^r q^n \pi_q^{m-r}. \quad (\text{A11})$$

The combination of  $\alpha=0$  and 1, corresponding to averaging by  $x + \chi^*$ , is the symmetric ordering of Eq. (32).  $\square$

*The product rule, proof of Eqs. (38) and (39):* The phase space function corresponding to the product of two operators  $\hat{F} = \hat{A}\hat{B}$ , by the definition of Eq. (36), is

$$\begin{aligned}
 F(q,p) &= \langle q | \hat{A} \hat{B} | p \rangle e^{-ipq/\hbar} = \int \langle q | \hat{A} | p' \rangle \langle p' | \hat{B} | p \rangle e^{-ipq/\hbar} dq dp \\
 &= \int A(q,p') B(q',p) \exp \frac{-i(q'-q)(p'-p)}{\hbar} dq dq', \quad (\text{A12})
 \end{aligned}$$

where by Eq. (36), we have substituted  $\langle q | \hat{A} | p' \rangle = A(q,p') \exp(ip'q/\hbar)$  and similarly for  $\langle q' | \hat{B} | p \rangle$ . With further change of variables  $q' - q = q''$  and  $p' - p = p''$ , we obtain

$$F(q,p) = \int A(q,p''+p) B(q''+q,p) e^{-iq''p''/\hbar} dq'' dp'' = \sum_{n=0}^{\infty} \frac{(-i\hbar)^n}{n!} \frac{\partial^n A(q,p)}{\partial p^n} \frac{\partial^n B(q,p)}{\partial q^n}, \quad (\text{A13})$$

where we have Taylor-expanded  $A(q,p+p'')$  and  $B(q+q'',p)$  about  $(q,p)$  and carried out the required integration by parts.

To deduce Eq. (39), we first Fourier-transform  $A(q,p)$  to  $a(p',q')$  and  $B(q,p)$  to  $b(p'',q'')$  in Eq. (A13) and carry out the necessary differentiations:

$$\begin{aligned}
 F(q,p) &= \sum_{n=0}^{\infty} \frac{(-i\hbar)^n}{n!} \frac{\partial^n}{\partial p^n} \int a(p',q') \exp \frac{-ip'q + iq'p}{\hbar} dp' dq' \frac{\partial^n}{\partial q^n} \\
 &\quad \times \int b(p'',q'') \exp \frac{-ip''q + iq''p}{\hbar} dq'' dp'' \\
 &= \int a(p',q') \exp \frac{-ip'q + iq'p}{\hbar} b(p'',q'') \exp \frac{-ip'',q''p}{\hbar} e^{-iq'p''/\hbar} dq' dp' dq'' dp''. \quad (\text{A14})
 \end{aligned}$$

Next we operate on Eq. (A14) by a Taylor-expanded form of  $U_\alpha$  as in Eq. (A2) and perform the required differentiations:

$$\begin{aligned}
 F_\alpha(q,p) &= U_\alpha F(q,p) = \int e^{i\alpha q'p'/\hbar} \exp \frac{-ip'q + iq'p - (1-\alpha)q'p'' + \alpha q''p'}{\hbar} a(q',p') \\
 &\quad \times e^{i\alpha q''p''/\hbar} \exp \frac{-ip''q + iq''p}{\hbar} b(p'',q'') dq' dp' dq'' dp''. \quad (\text{A15})
 \end{aligned}$$

The exponentials preceding  $a(p',q')$  can be written as

$$e^{i\hbar\alpha^2/\partial p \partial q} \exp \frac{-ip'(q + \alpha q'') + iq'(p - (1-\alpha)p'')}{\hbar},$$

where the first factor is simply  $U_\alpha(q,p)$  independent of the integration variables  $(q',p',q'',p'')$ . With this provision integrations over  $q'$  and  $p'$  can now be carried out and  $a(p',q')$  inverse-Fourier transformed. One finds

$$F_\alpha(q,p) = \int \{U_\alpha A[q + \alpha q'', p - (1-\alpha)p'']\} e^{i\alpha q''p''/\hbar} e^{(-ip''q + iq''p)/\hbar} b(p'',q'') dq'' dp''. \quad (\text{A16})$$

We again apply the same trick. To the left of the rightmost exponential we replace, everywhere,  $q''$  by  $(-i\hbar \partial/\partial p)$  and  $p''$  by  $(i\hbar \partial/\partial q)$ , perform the inverse Fourier transform of  $b(p'',q'')$  and find

$$\begin{aligned}
F_\alpha(q,p) &= U_\alpha F(q,p) = A_\alpha \left[ q + i\hbar \alpha \frac{\partial}{\partial p}, p - i\hbar \alpha(1-\alpha) \frac{\partial}{\partial q} \right] B_\alpha(q,p) \\
&= \sum_{n=0}^{\infty} \frac{(i\hbar)^n}{n!} \left[ \alpha \frac{\partial}{\partial q_A} \frac{\partial}{\partial p_B} - (1-\alpha) \frac{\partial}{\partial p_A} \frac{\partial}{\partial q_B} \right]^n A_\alpha(q,p) B_\alpha(q,p). \quad (\text{A17})
\end{aligned}$$

where  $\partial/\partial p_A$  indicates a differentiation on  $A(q,p)$  only, similarly the other differential operators.  $\square$

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