International Journal of Modern Physics B, Vol. 7, No. 18 (1993) 3255–3272

A PHASE SPACE FORMULATION OF QUANTUM STATE FUNCTIONS*

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Received 3 July 1992
Revised 23 January 1993

Allowing for virtual paths in phase space permits an extension of Hamilton's principle of least action, of lagrangians and of hamiltonians to phase space. A subsequent canonical quantization, then, provides a framework for quantum statistical mechanics. The classical statistical mechanics and the conventional quantum mechanics emerge as special case of this formalism. Von Neumann's density matrix may be inferred from it. Wigner's functions and their evolution equation may also be obtained by a unitary transformation.

1. Introduction

The hamiltonian formalism of classical dynamics treats the coordinates, q, and momenta, p, on an equal basis. When it comes to quantization procedure, however, one either chooses a coordinate or momentum representation and ends up with state functions either in q or in p space. The equal status of q and p is lost. It is possible to keep the symmetry between canonical coordinates and momenta in the process of quantization and, at once, arrive at state functions in a phase space representation. In his pioneering work(1932), Wigner[1] uses conventional quantum mechanics as a bridge to the phase space problem. The characteristic function method of Moyal,[2] Hillary *et al.*,[3] Mehta[4] and others, also depart from the same tenet. See also Agarwal and Wolf,[5] Han *et al.*,[6] Kim and Wigner,[7] Jannussis *et al.*,[8] and references therein. The present paper begins from a somewhat different level of abstraction and aims directly at quantum mechanics in phase space. *Extended* lagrangians and hamiltonians in phase space are introduced in Sec. 2. The idea behind the extension is the virtual paths in phase space as opposed to those in configuration space. A quantization rule based on these extended entities is proposed in Sec. 3. This, in turn, leads to state functions in phase space and to an evolution equation most suited for quantum statistical mechanics. Two limiting cases are elaborated in Sec. 4. In the limit of zero Planck constant one recovers the distribution functions

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of classical statistical mechanics, satisfying Liouville's equation. In the limit of pure states one arrives at the conventional quantum mechanics. Von Neumann's density matrix is derived in Sec. 5. The logic behind it, however, is different. In particular, no need arises to postulate ensembles explicitly. Wigner's functions and equation are obtained by a canonical transformation on those of this paper. This is demonstrated in Sec. 6.

2. Review of Hamiltonian Dynamics and Generalization

Let $\mathcal{L}^q(q, \dot{q})$ be a lagrangian, where $q = \{q_i\}$ is the collection of the generalized coordinates specifying a system. A trajectory of the system in q space is obtained by solving the Euler-Lagrange equations for $q_i(t)$,

$$\frac{d}{dt}\frac{\partial \mathcal{L}^q}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}^q}{\partial q_i} = 0 \ . \tag{1}$$

The derivative $\partial \mathcal{L}^q / \partial \dot{q}_i$ calculated on an actual trajectory, that is, on a solution of Eq. (1), is the momentum conjugate to q_i. The same derivative calculated on a virtual orbit, not a solution of Eq. (1), exists. It may not, however, be interpreted as a canonical momentum. Let $H(p, q)$ be the hamiltonian. It is related to $\mathcal{L}^q$ through the Legendre transformation,

$$H\left(\frac{\partial \mathcal{L}^q}{\partial \dot{q}_i}, q\right) = \dot{q}_i \frac{\partial \mathcal{L}^q}{\partial \dot{q}_i} - \mathcal{L}^q(q, \dot{q}) \ . \tag{2}$$

For a given $\mathcal{L}^q$, Eq. (2) is an algebraic equation for H. One may, however, take a different point of view. For a given functional form of $H(p, q)$, Eq. (2) may be considered as a differential equation for $\mathcal{L}^q$. Its non unique solutions differ from one another by total time derivatives.

So much for the description of the system in configuration space. One may also study it in the momentum space. Let $\mathcal{L}^p(p, \dot{p})$ be a lagrangian in p representation. (See Goldstein,[9] 1980, p. 372, for this type of lagrangians). It is related to $H(p, q)$ as follows,

$$H\left(p, \frac{\partial \mathcal{L}^p}{\partial \dot{p}_i}\right) = -\dot{p}_i \frac{\partial \mathcal{L}^p}{\partial \dot{p}_i} + \mathcal{L}^q(p, \dot{p}) \ , \tag{3}$$

where the functional dependence of H on its argument is the same as in Eq. (2). In principle, Eq. (3) should be solvable for $\mathcal{L}^p$ up to an additive total time derivative term. Once $\mathcal{L}^p$ is known the actual trajectories in p space are obtainable from a Euler-Lagrange equation analogous to Eq. (1) in which q is replaced by p. The derivative $\partial \mathcal{L}^p / \partial \dot{p}_i$ along an actual p trajectory is the canonical coordinate conjugate to p_i. Calculated on a virtual orbit, it is not.

A third option is open. One may combine the two pictures and define an *extended* lagrangian in the phase space as the sum of p and q lagrangians,

$$\mathcal{L}(p, q, \dot{p}, \dot{q}) = -\dot{q}p - q\dot{p} + \mathcal{L}^q + \mathcal{L}^p \ , \tag{4}$$

where p and q, as is the tradition in phase space studies, are independent variables. The first two terms in Eq. (4) constitute a total time derivative. The equations of motion are

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = \frac{d}{dt}\frac{\partial \mathcal{L}^q}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}^q}{\partial q_i} = 0 \ , \tag{5a}$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{p}_i} - \frac{\partial \mathcal{L}}{\partial p_i} = \frac{d}{dt}\frac{\partial \mathcal{L}^p}{\partial \dot{p}_i} - \frac{\partial \mathcal{L}^p}{\partial p_i} = 0 \ , \tag{5b}$$

The two equations in (5) are uncoupled. Equation (5a) with initial data for q_i and $\dot{q}_i$, gives a q trajectory. Similarly, Eq. (5b) with arbitrary initial values for p_i and $\dot{p}_i$, gives a p trajectory. In order for the two orbits to represent the same state of motion, the initial data should be constrained to $p_i = \partial \mathcal{L}^q / \partial \dot{q}_i$ and $q_i = \partial \mathcal{L}^p / \partial \dot{p}_i$. In other words, p_i and q_i should initially be canonically conjugate pairs. It will be shown below that if p and q are canonically conjugate for one time they should remain so for all the time. A state of motion so constrained will be referred to as a *pure* state. The extended lagrangian is zero on a pure state. For, by Eqs. (2) and (3) and the conditions that p and q are canonically conjugate, one finds $\mathcal{L} = H(p, q) - H(p, q) = 0$. In general, however, an unconstrained solution of Eqs. (5) is, simply, two independent solutions in q and p representations. Such solutions will be referred to as *mixed* states. The nomenclature, pure and mixed, is borrowed from quantum statistical mechanics and, as we shall see later, they convey the same notions as therein. The extended lagrangian is non zero along a mixed state trajectory. A word of caution is in order. One may not infer a doubling of the number of degrees of freedom of the system, contrary to what the outlook of the extended lagrangian may suggest. Equations (4) and (5) simply carry the p and q representations of the motion side by side in a symmetrical way, a provision that will prove to be essential for a formulation of quantum mechanics in phase space. The concept behind the extension of lagrangians and the resulting equations of motion is simple to explain, though it is somewhat unorthodox. Hamilton's principle postulates minimum action along the actual trajectories in configuration space as compared with the action along neighboring virtual paths. In the extended form of these notions, one assumes minimum action along the actual trajectories in phase space and compares its value with those on virtual paths in the same space. For a virtual path in phase space there is a much larger choice than for those in q space. This point of view is elaborated in the Appendix.

Second canonization: The p and q in Eqs. (4) and (5) are not, in general, canonical pairs. They are so only on pure states and through a proper choice of the initial

values. This gives the freedom of introducing a second set of canonical momenta for both p and q. One does this through the extended lagrangian. Thus,

$$\pi_{qi} = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \frac{\partial \mathcal{L}^q}{\partial \dot{q}_i} - p_i \ , \tag{6a}$$

$$\pi_{pi} = \frac{\partial \mathcal{L}}{\partial \dot{p}_i} = \frac{\partial \mathcal{L}^p}{\partial \dot{p}_i} - q_i \ . \tag{6b}$$

Evidently, π_q and π_p vanish on pure state orbits and remain non zero on mixed ones. From these *extended* momenta, one defines an *extended* hamiltonian,

$$\mathcal{H}(p, q, \pi_p, \pi_q) = \pi_{qi}\dot{q}_i + \pi_{pi}\dot{p}_i - \mathcal{L}(p, q, \dot{p}, \dot{q}) \ . \tag{7}$$

To eliminate $\dot{q}$ and $\dot{p}$, one substitutes for $\mathcal{L}$ from Eq. (4), and for $\mathcal{L}^q$ and $\mathcal{L}^p$ from Eqs. (2) and (3), respectively. One then uses Eqs. (6) to eliminate $\partial \mathcal{L}^q/\partial \dot{q}_i$ and $\partial \mathcal{L}^p/\partial \dot{p}_i$ and arrives at

$$\begin{aligned} \mathcal{H}(p, q, \pi_p, \pi_q) &= H(p + \pi_q, q) - H(p, q + \pi_p) \\ &= \sum_{n=1} \frac{1}{n!} \left\{ \frac{\partial^n H}{\partial p^n} \pi_q^n - \frac{\partial^n H}{\partial q^n} \pi_p^n \right\} \ . \end{aligned} \tag{8}$$

Example: For $H = \frac{1}{2}p^2 + V(q)$, Eq. (8) gives

$$\mathcal{H} = \frac{1}{2}(p + \pi_q)^2 + V(q) - \frac{1}{2}p^2 - V(q + \pi_p) \ . \tag{9}$$

To see the implications of the extended hamiltonian let us write down the equations of motion:

$$\dot{p} = \frac{\partial \mathcal{H}}{\partial \pi_p} = -\left.\frac{\partial H}{\partial q}\right|_{p,\, q+\pi_p} , \tag{10a}$$

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial \pi_q} = \left.\frac{\partial H}{\partial p}\right|_{p+\pi_q,\, q} , \tag{10b}$$

$$\dot{\pi}_p = -\frac{\partial \mathcal{H}}{\partial p} = -\left.\frac{\partial H}{\partial p}\right|_{p+\pi_q,\, q} + \left.\frac{\partial H}{\partial p}\right|_{p,\, q+\pi_p} , \tag{11a}$$

$$\dot{\pi}_q = -\frac{\partial \mathcal{H}}{\partial q} = -\left.\frac{\partial H}{\partial q}\right|_{p+\pi_q,\, q} + \left.\frac{\partial H}{\partial q}\right|_{p,\, q+\pi_p} . \tag{11b}$$

One possible solution of Eq. (11) is $\pi_p = \pi_q = 0$. By Eqs. (6), this simply asserts that p and q are canonically conjugate pairs on this solution and remain so for all the time. Hence, Eqs. (10) reduce to the familiar Hamilton's equations of classical dynamics. These are the pure state solutions. There are other solutions with non vanishing π_p and π_q. These are the mixed state solutions, each consisting of two independent motions in q and p representations.

3. A Phase Space Quantization

Beside the q and p representations of quantum mechanics, many others have been entertained in the literature. See Bopp,[10] Aharonov,[11] Berezin *et al.*[12] and Jannussis *et al.*,[13] Kim *et al.*[6] and Ghosh *et al.*[14] In Berezin *et al.*'s notation all these may be summarized in the form of a commutation relation $[P, Q] = i\hbar$, where $P = \alpha_1 p + \beta_1 q + \gamma_1 \frac{\partial}{\partial p} + \delta_1 \frac{\partial}{\partial q}$ and $Q = \alpha_2 p + \beta_2 q + \gamma_2 \frac{\partial}{\partial p} + \delta_2 \frac{\partial}{\partial q}$, and α_i, β_i, γ_i and δ_i are appropriate constants. Our presentation below, in the final examination, comes close to the Jannussis[13] formalism. In his analysis one solves two Schrödinger's equations in a $q \otimes q$ space. In ours one does the same in a $p \otimes q$ space. Departing points in the two approaches, however, are different.

The Hilbert space: Let X be the function space of all square integrable complex functions, $X : \{\chi(p, q); \int \chi^* \chi dpdq < \infty\}$. The inner product in X is defined as

$$(\chi, \sigma) = \int \chi^* \sigma dpdq \; ; \quad \chi, \sigma \in X \; , \tag{12}$$

where dp and dq denote the volume elements of p and q spaces, respectively.

Postulates: a) p and q will be considered as independent c-number operators in X. For π_p and π_q, however, the differential operators and commutation brackets will be borrowed from the traditional quantum mechanics,

$$\pi_{qi} = -i\hbar \frac{\partial}{\partial q_i} \; , \quad [\pi_{qi}, q_j] = -i\hbar \delta_{ij} \; , \tag{13a}$$

$$\pi_{pi} = -i\hbar \frac{\partial}{\partial p_i} \; , \quad [\pi_{pi}, p_j] = -i\hbar \delta_{ij} \; . \tag{13b}$$

Note also the following

$$[p_i, q_j] = [p_i, p_j] = [q_i, q_j] = 0 \; , \tag{13c}$$

$$[\pi_{pi}, \pi_{qj}] = [\pi_{pi}, \pi_{pj}] = [\pi_{qi}, \pi_{qj}] = 0 \; . \tag{13d}$$

By virtue of Eq. (8), the extended hamiltonian, $\mathcal{H}(p, q, \pi_p, \pi_q)$, is also an operator in X . All these operators are hermitian.

b) A state function $\chi(p, q, t) \in X$ will be assumed to satisfy the following Schrödinger type equation

$$i\hbar\frac{\partial\chi}{\partial t} = \mathcal{H}\chi = \left\{H\left(p - i\hbar\frac{\partial}{\partial q}, q\right) - H\left(p, q - i\hbar\frac{\partial}{\partial p}\right)\right\}\chi$$
$$= \sum_{n=1}\frac{(-i\hbar)^n}{n!}\left\{\frac{\partial^n H}{\partial p^n}\frac{\partial^n}{\partial q^n} - \frac{\partial^n H}{\partial q^n}\frac{\partial^n}{\partial p^n}\right\}\chi \,. \tag{14}$$

c) The expectation value of an observable $f(p, q)$, a c-number operator in the present formalism, will be calculated from

$$\langle f\rangle = \int f(p, q)\chi^*(p, q)dpdq \,. \tag{15a}$$

Not all solutions of Eq. (14) are admissible state functions. Admissible ones: (a) should give real expectation values for observables, that is, for those $f(p, q)$'s whose operator equivalents, in either q and p representation, are hermitian, (b) should give positive values for positive observables, (c) in particular for $f = 1$, Eq. (15a) should give

$$\int \chi^* dpdq = 1 \,. \tag{15b}$$

Criteria for the realization of these conditions will be given in Sec. 5. Equation (15b) should not be confused with the norm $\int \chi^*\chi dpdq$. In fact, a state function satisfying Eq. (15b) may not, in general, have unit norm. The formalism presented by postulates a, b and c above is conjectured to be a formulation of quantum mechanics in phase space or of quantum statistical mechanics (apart from thermodynamic considerations). It contains the classical statistical mechanics and the traditional quantum mechanics as special cases. It also accommodates the well known density matrix formalism in a natural way. First, however, let us familiarize ourselves with Eq. (14).

Solutions of Eq. (14): Let

$$\chi(p, q, t) = F(p, q, t)e^{-ipq/\hbar} \,. \tag{16a}$$

This transformation is suggested by the total derivative added to the lagrangian of Eq. (4), $-d(pq)/dt$. The effect is the appearance of a phase factor, $\exp(-ipq/\hbar)$, in the state function that would have been in the absence of the total derivative. It is easily verified that

$$\left(p - i\hbar\frac{\partial}{\partial q}\right)\chi = -i\hbar\frac{\partial F}{\partial q}e^{-ipq/\hbar} \,, \tag{16b}$$

$$\left(q - i\hbar\frac{\partial}{\partial p}\right)\chi = -i\hbar\frac{\partial F}{\partial p}e^{-ipq/\hbar} \,. \tag{16c}$$

Substituting Eqs. (16) in Eq. (14) and eliminating the exponential factor gives

$$\left\{H\left(-i\hbar\frac{\partial}{\partial q}, q\right) - H\left(p, -i\hbar\frac{\partial}{\partial p}\right)\right\} F = i\hbar\frac{\partial F}{\partial t} . \tag{17}$$

Equation (17) has separable solutions of the form

$$F_{\alpha\beta}(p, q, t) = \psi_\alpha(q, t)\phi^*_\beta(p, t) , \tag{18a}$$

where

$$i\hbar\frac{\partial\psi_\alpha}{\partial t} = H\left(-i\hbar\frac{\partial}{\partial q}, q\right)\psi_\alpha , \tag{18b}$$

$$-i\hbar\frac{\partial\phi^*_\beta}{\partial t} = H\left(p, -i\hbar\frac{\partial}{\partial p}\right)\phi^*_\beta . \tag{18c}$$

Equation (18b), however, is the Schrödinger equation in q representation, and Eq. (18c) is the complex conjugate of the same in p representation. The α and β in Eqs. (18a) are not, in general, eigenindices, though this possibility is open. To $\psi_\alpha(q, t)$ there corresponds a Fourier transform $\phi_\alpha(p, t)$ and conversely

$$\psi_\alpha(q, t) = (2\pi\hbar)^{-N/2}\int \phi_\alpha(p, t)e^{ipq/\hbar}dp , \tag{19a}$$

$$\phi_\alpha(p, t) = (2\pi\hbar)^{-N/2}\int \psi_\alpha(q, t)e^{-ipq/\hbar}dq , \tag{19b}$$

where N is the number of degrees of freedom of the system, the dimensionality of p and q vectors.

Equations (14), (17) and (18) are linear. Hence a state function χ may be constructed by superposition:

$$\chi = a_{\alpha\beta}F_{\alpha\beta}e^{-ipq/\hbar} = a_{\alpha\beta}\psi_\alpha(q, t)\phi^*_\beta(p, t)e^{-ipq/\hbar} , \tag{20a}$$

$$a = a^\dagger, \text{ positive definite} ; \quad \text{tr } a = 1 , \tag{20b}$$

where summation over repeated indices is implied. The reason for limiting the matrix of the expansion coefficients to positive definite hermitian matrices is to guarantee the conditions set forth for the admissibility of χ in the paragraph following Eq. (15a). We will return to this point in Sec. 5.

Some useful properties of χ: It was noted earlier that $\psi_\alpha(q, t)$ and $\phi_\alpha(p, t)$ are mutually Fourier transforms and are related through Eqs. (19). Integrating

Eq. (20a) over p or q gives

$$(2\pi\hbar)^{-N/2}\int \chi(p, q, t)dp = a_{\alpha\beta}\psi_\alpha(q, t)\psi^*_\beta(q, t)\ , \tag{21a}$$

$$(2\pi\hbar)^{-N/2}\int \chi(p, q, t)dq = a_{\alpha\beta}\phi_\alpha(p, t)\phi^*_\beta(p, t)\ . \tag{21b}$$

Furthermore, if the sets $\{\psi_\alpha(q, t)\}$ and $\{\phi_\alpha(p, t)\}$ are orthonormal ones, one obtains

$$\int \chi^*\chi dp = (a^\dagger a)_{\alpha\gamma}\psi^*_\alpha(q, t)\psi_\gamma(q, t)\ , \tag{22a}$$

$$\int \chi^*\chi dq = (a^\dagger a)_{\beta\gamma}\phi_\beta(p, t)\phi^*_\gamma(p, t)\ . \tag{22b}$$

The normalization condition for χ, is

$$(\chi, \chi) = \int \chi^*\chi dpdq = \mathrm{tr}(a^\dagger a) = 1\ . \tag{23}$$

This condition, however, will be abandoned in favor of tr $a = 1$ to ensure the more useful requirement of Eq. (15b).

Eigensolutions of Eq. (14): Let $\{E_n, \psi_n(q)\}$ and $\{-E_m, \phi^*_m(p)\}$ be the set of eigensolutions of Eqs. (18). Hereafter, Latin indices will denote eigensolutions. Otherwise the Greek indices will be used.

- The eigenvalues and eigenfunctions of Eq. (14) are $(E_n - E_m)$ and $\chi_{nm}(p, q) = \psi_n(q)\phi^*_m(p)\exp(-ipq/\hbar)$, respectively. Each eigenfunction has an associated time factor $\exp[-i(E_n - E_m)t/\hbar]$. The proof is a matter of substitution in Eq. (14).
- The zero eigenvalue has all χ_{nn}, $n = 1, 2, \ldots$ as eigenfunctions and is infinitely degenerate. All $\chi_{nn'}$s, $n \neq n'$ are time dependent.
- $\int \chi_{nm}(p, q)dpdq = \delta_{nm}$.
  Proof: $\int \psi_n\phi^*_m e^{-ipq/\hbar}dpdq = \int \psi_n\psi^*_m dq = \delta_{nm}$.

The properties above also hold for the solutions of classical Liouville's equation[15] and of Wigner's equation.[1,2] This is not a coincidence. We shall shortly see that Liouville's equation is a special case of Eq. (14) and Wigner's equation can be obtained from Eq. (14) by a unitary transformation.

4. Correspondence Principles

In this section two limiting cases of the proposed phase space quantization are explored. (a) The limit of classical statistical mechanics and (b) that of the conventional quantum mechanics. It will be seen that the main axioms of these two disciplines are contained in those of the present formalism.

I. **The classical correspondence:** Dividing Eq. (14) by $i\hbar$ and letting $\hbar \to 0$ gives

$$\partial\chi/\partial t + \{\chi, H\} = 0 , \tag{24}$$

where $\{\ldots\}$ is a Poisson bracket. Equation (24), however, is Liouville's equation that lies at the foundation of equilibrium and nonequilibrium classical statistical mechanics. Its real and positive solutions are interpreted as classical probability densities. In general, however, Eq. (24) has complex and non positive solutions. Alone, they may not be used as probability densities. See Prigogine[16] and Sobouti.[15] Two features of the present derivation is noteworthy. 1) Nowhere in quantum mechanics, and the classical limits $\hbar \to 0$ inferred in as lucid a way as Eq. (24) is obtained, a remark that has also been made by Snygg[17] for Wigner's evolution equation. More worthy of contemplation, however, is the notion of probability that has crept into Eq. (24) through the commutation rules of Eqs. (13). It stands in contradistinction with what one finds in the classical derivation of Liouville's equation. In statistical mechanical theories one considers a system of many degrees of freedom. One is usually not capable of or interested in knowing all details of the system. Hence, one creates an ensemble of such systems, assigns a probability $\rho(p, q, t)$ to each state (p, q), and proceeds to calculate ensemble average of the dynamical quantities. This notion of probability is a matter of choice by the observer. It could be avoided if the observer is prepared to spare sufficient patience and computing capabilities. It does not stem from an inherent limitation put forward by nature, of the sort that one encounters in quantum mechanics, that prevents precise and simultaneous determination of non commuting observables. On the other hand, Eq. (24) is derived from a quantum principle, from Eq. (14) which itself is based on the uncertainty principles implied by Eqs. (13). There is no notion of ensemble in Eq. (24). Perhaps one could say that the statistical aspect of the classical statistical mechanics has a quantum origin. And if so, it should be accepted as an inherent inhibition by nature on the way of precise data acquisition?

II. **The quantum correspondence:** A single term from Eqs. (20), $\chi = \psi_\alpha \phi_\alpha^* \exp(-ipq/\hbar)$, corresponds to what is called a pure state in quantum statistical mechanics. It gives the same amount of information as the quantum mechanical description of the system in $\psi_\alpha(q,t)$ state. One may verify this by examining the following instances.

- Using Eq. (19a) to perform integrations over p, one easily finds $(2\pi\hbar)^{-N/2} \int \chi dp = \psi_\alpha^* \psi_\alpha$; that is, irrespective of what goes on in p space the probability density in q space is identical with that of the conventional quantum mechanics. Similarly $(2\pi\hbar)^{-N/2} \int \chi dq = \phi_\alpha^* \phi_\alpha$, with a similar interpretation.
- The uncertainty principle in its standard form, $\Delta p_i \Delta q_i \geq \hbar$, holds. **Proof**: From Eq. (15) one finds

$$(\Delta q_i)^2 = (2\pi\hbar)^{-N/2} \int (q_i - \bar{q}_i)^2 \chi^* dpdq = \int \psi_\alpha^* (q_i - \bar{q}_i)^2 \psi_\alpha dq , \tag{25a}$$

where $\bar{q}_i$ is the expectation value of q_i. Equation (19a) is used to perform integration over p. For Δp_i one similarly finds

$$(\Delta p_i)^2 = (2\pi\hbar)^{-N/2} \int (p_i - \bar{p}_i)^2 \chi^* dpdq = \int \psi_\alpha^* \left(-i\hbar \frac{\partial}{\partial q} - \bar{p}_i\right)^2 \psi_\alpha dpdq \ , \tag{25b}$$

where again we have substituted for ϕ_α^* in terms of its Fourier transform and carried out the integration over p. With Δq and Δp given by Eq. (25) the proof of the uncertainty principle can be found in standard quantum mechanical literature.[18]

- For the expectation value of any $Q(q)$ one finds

$$\langle Q \rangle = (2\pi\hbar)^{-N/2} \int Q \psi_\alpha^* \phi_\alpha e^{ipq/\hbar} dpdq = \int \psi_\alpha^* Q \psi dq \ . \tag{26a}$$

- For p_i^m one finds

$$\langle p_i^m \rangle = (2\pi\hbar)^{-N/2} \int p_i^m \psi_\alpha^* \phi_\alpha e^{ipq/\hbar} dpdq$$

$$= \int \psi_\alpha^* \left(-i\hbar \frac{\partial}{\partial q_i}\right)^m \psi_\alpha dq \ . \tag{26b}$$

- For functions $P(p)Q(q)$, where each factor is expressed as convergent power series or polynomials in their respective arguments one obtains

$$\langle PQ \rangle = \int \psi_\alpha^* Q(q) P\left(-i\hbar \frac{\partial}{\partial q}\right) \psi_\alpha dq \ . \tag{26c}$$

The proof proceeds along the lines for Eqs. (26a) and (b).

There is a noteworthy feature to the averaging rules expressed by Eq. (26c). No matter how the factors $P(p)$ and $Q(q)$ are arranged initially in a product, the averaging procedure decides on its own unambiguous ordering: $Q(q)P(-i\hbar\partial/\partial q)$. In other words, P and Q as operators do not operate on each other in the process of averaging. This so-called standard ordering, is to be expected and indicates a logical consistency in the present formulation. For, the averaging rules of Eqs. (26) are obtained from that of Eq. (15) in phase space representation. Any operator $f(p, q)$ is a c-number in this formulation. The variables p and q are independent and do not interfere with each other.

5. Quantum Statistical Mechanics

Finally we come to the main theme of this paper: that the phase space quantization is a proper framework for quantum statistical mechanics. Traditionally one formulates the quantum statistics by introducing a density matrix or density operator for the so-called mixed quantum states of an ensemble of systems and proceeds to calculate averages of the dynamical quantities over both the quantum states of a

system and over ensembles of such systems. In what follows it is shown that the usual density matrix theory of mixed quantum states can be reproduced from the present formalism. The logic behind it, however, does not require to postulate an ensemble of identical systems explicitly.

5.1. Density matrix in phase space quantization

Let

$$\{\chi_{mn}(p, q) = \psi_m(q)\phi_n^*(p)e^{-ipq/\hbar}\} \in X \tag{26d}$$

be an orthonormal basis for the Hilbert space, X, defined in Sec. 3, where ψ_m and ϕ_m are mutually Fourier transforms. Orthonormality relations are $(\psi_m, \psi_k) = \delta_{mk}$, $(\phi_n, \phi_\ell) = \delta_{n\ell}$, and $(\chi_{mn}, \chi_{k\ell}) = \delta_{mk}\delta_{n\ell}$. Only completeness, and orthonormality of $\{\chi_{mn}\}$, $\{\psi_m\}$ and $\{\phi_n\}$ are of interest. They are not required to satisfy Eqs. (14) or (18), though this is a possibility. A state function $\chi(p, q, t)$ may be expanded as

$$\chi = a_{mn}(t)\chi_{mn}(p, q) \ . \tag{27a}$$

$$a(t) = \text{hermitian and positive definite} \ ; \quad \text{tr } a = 1 \ . \tag{27b}$$

Differentiating Eq. (27a) with respect to time and using Eqs. (14), (16) and (18) gives

$$\begin{aligned} i\hbar\dot{\chi} &= i\hbar\dot{a}_{mn}\psi_m\phi_n^* e^{-ipq/\hbar} \\ &= a_{mn}\left\{H\left(-i\hbar\frac{\partial}{\partial q}, q\right)\psi_m\phi_m^* - \psi_m H\left(p, i\hbar\frac{\partial}{\partial p}\right)\phi_m^*\right\} e^{-ipq/\hbar} \ . \end{aligned} \tag{28}$$

Multiplying Eq. (28) by $\chi_{\ell k}^*$, integrating over the phase space, and using the orthogonality of $\{\chi_{mn}\}$, $\{\psi_m\}$, and $\{\phi_n\}$ gives

$$i\hbar\dot{a} = [H, a] \ ; \quad a = a^\dagger \text{ and positive definite} \ , \tag{29}$$

where H is now the hermitian matrix of the hamiltonian with elements $H_{\ell m} = (\psi_\ell, H, \psi_m) = (\phi_\ell, H\phi_m) = H_{m\ell}^*$. Equation (29) is von Neumann's equation for the density matrix. Next we examine the averaging procedure with a.

5.2. *Expectation values*

From Eq. (15a), for a simple c-number power function $f = p^j q^i$, one obtains

$$\begin{aligned} \langle q^i p^j\rangle = \langle p^j q^i\rangle &= (2\pi\hbar)^{-N/2} a_{mn}^* \int \psi_m^*(q)\phi_n(p)e^{ipq/\hbar} q^i p^j \, dpdq \\ &= a_{mn}^* \int \psi_m^* q^i \left(-i\hbar\frac{\partial}{\partial q}\right)^j \psi_n \, dq \\ &= a_{mn}^*(q^i p^j)_{mn} = \text{tr}(a^\dagger f) \ . \end{aligned} \tag{30a}$$

The second equality in Eq. (30) is obtained from defining Eq. (15a), the third by performing the p integrations by the known Fourier transform techniques. The fourth equality uses the conventional notation for the matrix elements of $f = q^i p^j$. Here, once more one encounters the standard ordering for powers of q and $\partial/\partial q$. Generalization of Eq. (30) for an arbitrary observable is straightforward. Let $f(q, p)$ have a convergent power series expansions of the form $f(q, p) = b_{ij} q^i p^j$ The matrix elements of f and its expectation values, will be

$$f_{nm} = \int f \chi^*_{nm} dp dq \tag{30b}$$

$$\langle f \rangle = \mathrm{tr}\,(a^\dagger f)\ . \tag{30c}$$

5.3. *Admissible state functions*

The only use of a state function is in the evaluation of the averages of dynamical observables. Its properties should also be sought in this and only in this context. (1) Expectation values of an observable f with a corresponding hermitian matrix should be real. This requires a in Eq. (30) to be hermitian. (2) Expectation values of a positive definite observable f should be positive definite. This further restricts a to positive definite matrices. (3) For $f = 1$, Eq. (30) should give tr $a = 1$. This completes the list of the constraints on the matrix of expansion coefficients in Eqs. (20) and (27). In particular $\chi(p, q, t)$ is not even required to be real, let aside its positivity. From this point of view the usage of the word "probability density" in phase space quantization becomes a matter of semantics. For, distribution functions are expected to give averages over the entire region of the phase space and not over portions of it. They are not required to serve any other purpose. The argument for the positivity of a is taken from Glauber.[19]

5.4. *Comparison with von Neumann's density matrix of ensemble theories*

Let $\{\psi_m(q)\}$ denotes an orthogonal and complete set of the state functions of a quantum system in q representation. In an ensemble of such systems let $\psi^k(q, t) = A^k_m(t)\psi_m(q)$ be a state function of the kth member of the ensemble. The quantum and ensemble average of an observable $f(q, p)$ is written as

$$\langle f \rangle = \frac{1}{K}\sum_k (\psi^k, f\psi^k) = \frac{1}{K}\sum_k A^{k*}_m A^k_n \int \psi^*_m f \psi_n dq = \mathrm{tr}(af)\ , \tag{31}$$

where K is the number of systems in the ensembles, $a = \frac{1}{K}\sum_k A^k A^{k\dagger}$ is the usual density matrix of ensemble theories, and A^k is the column vector of expansion coefficients in $\psi^k(q, t)$. It is hermitian, positive definite, has unit trace, and satisfies Eq. (29) (see, e.g., Pathria,[20] Balescu[21] for further details). Thus, $a = A^\dagger A/K$ is entirely equivalent to that of Eqs. (27).

There are differences, however. In ensemble theories two notions of averaging are involved, one over ensemble members and the other over quantum states. These are explicitly displayed in Eq. (31). As was pointed out in the classical correspondence limit, Sec. 4, ensemble averaging and the probability assigned to ensemble members have origin in the practical limitations of the observer to attend to all details of the many parameter systems. This, in principle, should be avoidable by improving the capabilities of the observer. In contrast, the quantum averaging and the probabilistic origin of it are unavoidable and reflect an inherent reluctance of the nature to reveal precise information beyond what is permitted by the uncertainty principle. There are also two concepts of averaging and probability in the phase space formulation, one over the q space, the other over its Fourier replica, the p space. Both of these, however, are introduced through quantum principles, the pair of commutation relations of Eqs. (13) and the pair of uncertainty relations inherent in them. Could it be that the probabilities and averaging procedures associated with ensembles also have a quantum origin and should not be attributed to practical limitations?

5.5. *Wigner's functions*

A simple canonical transformation on p, q, π_p, π_q reproduces Wigner's formulation of phase space distribution functions. Let

$$p \to p + \delta\lambda\pi_q \ , \quad \pi_p \to \pi_p \ , \tag{32a}$$

$$q \to q + \delta\lambda\pi_p \ , \quad \pi_q \to \pi_q \ , \tag{32b}$$

where $\delta\lambda \ll 1$. The generator of this infinitesimal canonical transformation is (see Goldstein,[9] for notation and concepts)

$$G = \pi_p\pi_q = -\hbar^2\frac{\partial^2}{\partial p\partial q} \ , \tag{33a}$$

where the second equality is the operator form of the generator. For a finite λ, the transformation operator is[18]

$$U = e^{-\lambda G/i\hbar} = e^{-i\lambda\hbar\partial^2/\partial p\partial q} \ , \quad U^\dagger U = 1 \ . \tag{33b}$$

The case $\lambda = -1/2$ is interesting. It transforms the present evolution equation and phase space distributions to those of Wigner. The hamiltonian of Eq. (9) transforms into

$$\mathcal{H}' = U\mathcal{H}U^\dagger = \frac{1}{2}\left(p + \frac{1}{2}\pi_q\right)^2 + V\left(q - \frac{1}{2}\pi_p\right) - \frac{1}{2}\left(p - \frac{1}{2}\pi_q\right)^2 - V\left(q + \frac{1}{2}\pi_p\right) \ . \tag{34a}$$

The second equality here can actually be obtained by a simple substitution of Eqs. (32), for $\delta\lambda = -1/2$, in the classical expression of Eq. (9). A state function $\chi(p, q, t)$ transforms into

$$W(p, q, t) = U\chi(p, q, t) = e^{(1/2)i\hbar\partial^2/\partial p\partial q}\chi(p, q, t) \ . \tag{34b}$$

Multiplying Eq. (14) by U and using Eq. (34a), in its Taylor expanded form, and (33b) gives

$$\frac{\partial W}{\partial t} = -p\frac{\partial W}{\partial q} + \sum_{n=0} \frac{1}{(2n+1)!}\left(\frac{\hbar}{2i}\right)^{2n} \frac{\partial^{2n+1}V}{\partial q^{2n+1}}\frac{\partial^{2n+1}W}{\partial p^{2n+1}} \ . \tag{34c}$$

For $\chi_{\alpha\beta} = \psi_\alpha(q)\phi^*_\beta(p)e^{-ipq/\hbar}$, Eq. (34b) reduces to

$$W_{\alpha\beta}(p, q) = \int \psi_\alpha\left(q + \frac{1}{2}\hbar\tau\right)\psi^*_\beta\left(q - \frac{1}{2}\hbar\tau\right)e^{-ip\tau}d\tau \ , \tag{34d}$$

where time dependence is suppressed. Equation (34d) is Wigner's distribution functions.[1] Wigner derived Eq. (34c) by arguing that ψ's in Eq. (34d) are solutions of Schrödinger's equation. Moyal[2] reproduced Wigner's functions and equation, however, by a different approach, by an intricate manipulation of characteristic functions and Fourier transform properties. Moyal also showed the equivalence of Eqs. (34b) and (34d).[2] Arponen and Bishop[22] point out that Moyal's method is an example of the modern deformation theory. It should be noted that a unitary transformation of Eq. (34b) changes the averaging rule. In Eq. (15a) substitution for χ^* from Eq. (34b), gives $\langle f\rangle_{\chi^*} = \langle Uf\rangle_W$. That is, the expectation value of $f(p, q)$ with χ^* is only equal to the expectation value of $Uf(p, q)$ with W.

Derivation of Wigner's formulation of quantum distribution functions from the unitary transformations of Eq. (34b) indicates the possibility of a host of other unitary transformations. They are not, however, entirely equivalent; it is a common knowledge that different phase space functions imply different ordering rules for non commuting observables in quantum mechanics. See Shewell[23] for a list of such rules and criticisms. See also Mehta[4] and Agarwal and Wolf[5] for extensive discussions and further references on the subject. For example, Wigner's distributions imply Weyl's symmetrization rule,[2,5] while those of the present paper, as shown in Eq. (26c), are compatible with the standard ordering. Of course, the final verdict, on whether one or the other is preferable should come from observations involving products of non-commuting observables. In the absence of such evidence, however, the authors' argument in favor of χ function is the consistency arguments raised in the closing paragraph of Sec. 4, that is, p and q as phase space variables are independent; in their operator form they should leave each other alone.

The transformation of Eq. (31), however, is unique in one respect. It leads to a real evolution equation with possible real solutions. Evidently, this was much appreciated in the early attempts to compare Wigner's distribution functions with

the classical probability densities. The latter are real and positive throughout the accessible region of the phase space. Positivity of Wigner's functions is not realized, a point that has often been considered a weakness. From the point of view taken in this paper, however, this need not be so. The criteria for Wigner's functions to be admissible distributions could be the same as for χ^*'s.

Admissibility of negative or complex state functions is also pointed out by others. Mehta,[4] in his investigation of different phase space state functions and the ordering rule associated with each representation, concludes that: "The distribution functions may not only be negative, but may even be complex ... . Thus, we see that if negative and complex probabilities are admitted ... such a description is completely equivalent to the quantum mechanical discription".

6. Concluding Remarks

The new conceptual element in the proposed formalism is the consideration given to virtual paths in phase space. Once this is accepted, the procedure of second canonization, definition of extended lagrangian, $\mathcal{L}(p, q, \dot{p}, \dot{q})$, of second momenta, π_p and π_q, and of the extended hamiltonian, $\mathcal{H}(p, q, \pi_p, \pi_q)$, may proceed parallel to those of the conventional concepts. Quantization rules of Eqs. (13), the state functions χ, their use and evolution, also have precedence in the q space quantum mechanics.

From a pedagogical point of view the following are noteworthy. a) The unifying aspect : The classical statistical mechanics, the conventional quantum mechanics, the density matrix theory, and Wigner's distribution functions are brought under one and the same umbrella. b) The state functions of Eqs. (20) or (27) have simple forms and are easy to work with. It may be said that they are complex valued and may not be interpreted as probability densities, in the same way that Wigner's negative valued functions may not be. There is no need for such interpretation. It was argued that the only use of state functions was to calculate expectation values of dynamical variables. It is sufficient that they yield real values for observable functions, real positive values for positive observable functions and 1 for the unit function. c) Most students of physics become conversant in quantum mechanical parlance rather early in their career. The situation is not so with classical and quantum statistical mechanics. This, perhaps, could be traced to the somewhat abstract concept of ensembles. The formalism of this paper does not require much beyond the usual skills and techniques of quantum mechanics and are easy to master.

No statistical mechanics is complete without an underlying thermodynamics. The theory developed so far is an initial value problem. Given an acceptable $\chi(p, q, t = 0)$, the state function $\chi(p, q, t)$ may be obtained from Eqs. (20) or (27) by determining the matrix of the expansion coefficients. For a system of many degrees of freedom, however, it is not practical to give a detailed state function at some instant. This is true for the present equation of evolution, Eq. (14), and for Liouville's and von Neumann's equation. Customarily, the dilemma is solved by

brushing aside the question of initial values and inviting in a principle of maximum entropy in the course of evolution. Through this principle the expansion coefficients may then be determined. A formulation of entropy principle for the present phase space quantization will be presented elsewhere.

Appendix

Virtual paths in phase space: To develop a feeling for the extended lagrangian and hamiltonian and the concept behind them let us look at the variational foundation of the Euler-Lagrange equations. By Hamilton's principle one assumes that the action integral, $I = \int_{t1}^{t2} \mathcal{L}(q, \dot{q})dt$, is minimum along an actual trajectory in q space, the qt-plane of Fig. 1. To derive the law of motion, one considers virtual paths in the infinitesimal neighborhood of the actual one, calculates the corresponding infinitesimal change in the action in terms of the deviations, $\delta q(t) = q_{\rm vir}(t) - q_{\rm ac}(t)$, between the actual and virtual paths, and requires the first order variation in action to vanish. This definition of δq associates with each point of the virtual path a neighboring point on the actual one, situated on the line t = constant. See Fig. 1. Hence one concludes $\delta\dot{q}(t) = d\delta q/dt$, substitutes it in the action integral and integrates by parts to obtain

$$\delta I = \int_{t1}^{t2} \left(-\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} + \frac{\partial \mathcal{L}}{\partial q} \right) \delta q dt = 0 \, .$$

One then argues that δq is arbitrary. The integrand should vanish, giving the Euler-Lagrange equation. The rule for associating pairs of neighboring point, however, may be changed arbitrarily. For example, let us define $\delta q'(t) = q_{\rm vir}(t) - q_{\rm ac}(t+\epsilon(t)) = \delta q(t) - \epsilon\dot{q}_{\rm ac}(t)$ where $\epsilon(t)$ is infinitesimal and $\epsilon(t_1) = \epsilon(t_2) = 0$; see Fig.1. Otherwise

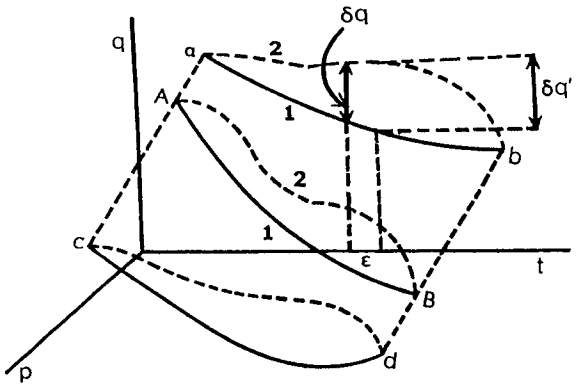

Fig. 1. Trajectories in pqt diagram. a1b and a2b are actual and virtual paths in q-space, respectively. A1B and A2B are actual and virtual paths in phase space, respectively. Projections of A1B and A2B on qt-plane are a1b and a2b, respectively.

$\epsilon(t)$ is arbitrary. For $\delta\dot{q}'$ one now finds

$$\delta\dot{q}' = \frac{d}{dt}\delta q - \frac{d}{dt}(\epsilon\dot{q}) \neq \frac{d}{dt}\delta q' \ .$$

For a given $\delta q(t)$ and, hence a given $\delta\dot{q}(t)$, one may vary $\delta\dot{q}'$ by assigning arbitrary values and functional forms for $\epsilon(t)$. This example indicates the possibility of accommodating a much larger class of variations in the variational derivation of equations of motion. In this particular example one obtains

$$\delta I = \int_{t1}^{t2}\left(-\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{q}} + \frac{\partial\mathcal{L}}{\partial q}\right)\delta q dt + \int_{t1}^{t2}\left(-\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{q}} + \frac{\partial\mathcal{L}}{\partial q}\right)\dot{q}\epsilon dt \ ,$$

which leads to the same equation of motion as it should be.

The extended lagrangian, $\mathcal{L}(p, q, \dot{p}, \dot{q})$, is designed to take this larger class of virtual variations into consideration by treating p and q as independent variables. Let us look at paths in phase space in pqt-diagram of Fig. 1. The solid curve AB is an actual trajectory in phase space, whose projection on qt-plane, solid ab, is the same actual q-space trajectory. The dashed curve AB is a virtual path in phase space whose projection on qt plane, dashed ab, is the same q space virtual path. Now, let us consider the semi cylindrical surface $abcd$ generated by translating the virtual path AB parallel to p axis. All virtual paths on this semi cylinder, that begin from A and end at B have the same projection, virtual ab, on qt plane. All are treated as a single virtual path in the conventional derivation of Euler-Lagrange equation. These paths have identical $\delta q(t)$ but differ in their $\delta p(t) = p_{\rm vir}(t) - p_{\rm ac}(t)$. This freedom of arbitrary virtual variations in p is possible only with phase space trajectories and through the extended lagrangian. Of course, the classical equation of motion obtained from the extended lagrangian are identical with those obtained from the ordinary lagrangian $\mathcal{L}(q, \dot{q})$. This is demonstrated in Eq. (5) in lagrangian formalism and in Eqs. (10) and (11) in hamiltonian formalism. The quantum implications of the extension, however, are dramatic, the least being the emergence of a unified view of classical statistical mechanics, quantum mechanics and statistical quantum mechanics.

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