On the relation between classical and quantum-thermodynamic entropy

Gian Paolo Beretta
Massachusetts Institute of Technology, Room 3-339, Cambridge, Massachusetts 02139

(Received 31 March 1983; accepted for publication 20 May 1983)

We discuss the unresolved problem of proving rigorously that in the classical limit $\hbar \to 0$, the quantum-thermodynamic entropy functional tends to the classical entropy functional. We state rather restrictive conditions that define the general problem of finding a complete classical phase-space representation of quantum kinematics. Whether the problem admits of solutions remains an unresolved question. We discuss a physically interesting attempt to relate the structure in the classical limit $\hbar \to 0$ of the well-known Blokhintzev, Wigner, and Wehrl phase-space functions to the spectral expansion of the quantum state operator.

PACS numbers: 05.30. – d, 02.50. + s

I. INTRODUCTION: PHYSICAL CONTEXT OF THE PROBLEM

The purpose of this paper is to discuss the problem of proving that in the classical limit $\hbar \to 0$ the quantum-thermodynamic entropy functional

$$s(\rho) = -k \operatorname{Tr} \rho \ln \rho \tag{1}$$

tends to the classical entropy functional

$$s^{\rm cl}(w) = -k \int \frac{dq\,dp}{2\pi\hbar}\, w(q,p) \ln w(q,p), \tag{2}$$

where ρ is the quantum state operator and w a properly defined classical state function. As recently stated by Wehrl,[1] "It is usually claimed that in the limit $\hbar \to 0$, the quantum-mechanical expression tends towards the classical one, however, a rigorous proof of this is nowhere found in the literature."

In this paper, we state conditions that define the problem of finding a classical phase-space representation of quantum kinematics. One such condition is that a properly defined classical state function w (the definition of which may involve limits as $\hbar \to 0$) should be such that $s^{\rm cl}(w) = s(\rho)$. Whether the problem thus defined admits of solutions remains an unresolved question which is worth further investigations. We gain some insight in the problem by studying the phase-space structure induced in the classical limit by the spectral expansion of the quantum state operator.

Our interest in this problem arises for physical reasons essentially distinct from the traditional. Indeed, even the physical meaning that we assign to the mathematical objects, especially ρ and w, is entirely different from the conventional. In our attempts to unify the laws of quantum mechanics and thermodynamics into a quantum thermodynamics,[2,3] an underlying hypothesis has been that no layer of statistical or information-theoretic reasoning should be required to bridge the gap between mechanics and thermodynamics. Indeed, in our theory there is no such gap. Quantum thermodynamics is a nonstatistical theory concerned exclusively with a causal description of the individual quantum states of a system, including a single particle.

A most important fundamental hypothesis[2] of quantum thermodynamics is that the general mathematical representation of the individual quantum states of a single isolated system cannot be in terms of the traditional state vectors $|\psi\rangle$ in the Hilbert space $\mathscr{H}$ of the system, but must be in terms of self-adjoint, nonnegative-definite, unit-trace operators ρ on $\mathscr{H}$ that are not necessarily idempotent. State operators ρ have the same mathematical properties ($\rho^\dagger = \rho$, $\rho \geqslant 0$, $\operatorname{Tr}\rho = 1$) as the statistical or density operators considered in traditional (von Neumann) quantum statistical mechanics.[4] But in quantum thermodynamics, their physical meaning is entirely different. The operators ρ represent individual states of a single system and not the index of statistics from a generally heterogeneous ensemble of identical systems. Thus, for example, the entropy functional $s(\rho)$, defined by Eq. (1), represents the entropy[5] of the single system in any of its states, equilibrium and nonequilibrium, dissipative and nondissipative,[3] and not a measure of statistical or information-theoretic uncertainty.

With this background, the problem of studying the classical limit $\hbar \to 0$ acquires for us a special physical meaning. The phase-space functions $w(q,p)$ represent individual classical states of a single system and not the index of statistics from a Gibbsian ensemble. The functional $s^{\rm cl}(w)$ represents the individual classical entropy of the single system in any of its classical states, and not the Gibbsian index of probability of phase.

However, we wish to emphasize that all the mathematical observations reported in this paper may obviously be interpreted also in the traditional way.

We restrict our discussion to the case of a single degree of freedom (e.g., a one-dimensional harmonic oscillator) so that the Hilbert space is $\mathscr{H} = L^2(\mathbb{R})$ and the classical phase space is $\Omega = \mathbb{R}^2$.

The paper is organized as follows. Coherent states and three well-known phase-space maps are briefly reviewed in Sec. II, conditions defining a complete phase-space representation of quantum kinematics are given in Sec. III, a discussion on the classical limit of the three phase-space maps is given in Sec. IV, and conclusions in Sec. V.

II. COHERENT STATES AND PHASE-SPACE FUNCTIONS

We denote the position and momentum operators by Q and P ($[Q,P] = i\hbar I$), and their eigenvalues by q and p so that $Q|q\rangle = q|q\rangle$ and $P|p\rangle = p|p\rangle$. The annihilation and creation

 0022-2488/84/051507-04$02.50

operators Z and $Z^\dagger$ ($[Z, Z^\dagger] = I$) are then defined by the relations[6]

$$Z \equiv \sqrt{1/2\hbar\omega}(\omega Q + iP), \quad Q = \sqrt{\hbar/2\omega}(Z^\dagger + Z),$$
$$Z^\dagger \equiv \sqrt{1/2\hbar\omega}(\omega Q - iP), \quad P = \sqrt{\omega\hbar/2}i(Z^\dagger - Z). \tag{3}$$

We call the normalized eigenvectors $|z\rangle$ of Z ($Z|z\rangle = z|z\rangle$) coherent vectors with "natural frequency" ω. For each eigenvalue z of Z, we define the real variables x and y (with dimensions of position and momentum, respectively) by the relations

$$x \equiv \sqrt{\hbar/2\omega}(z^* - z), \quad z = \sqrt{1/2\hbar\omega}(\omega x + iy),$$
$$y \equiv \sqrt{\omega\hbar/2}i(z^* + z), \quad z^* = \sqrt{1/2\hbar\omega}(\omega x - iy). \tag{4}$$

The representation of coherent vector $|z\rangle$ in configuration space is

$$\langle q|z\rangle = (\omega/\pi\hbar)^{1/4} \times \exp[-\omega(x-q)^2/2\hbar + iyq/\hbar - ixy/2\hbar], \tag{5}$$

whereas in momentum space it is

$$\langle p|z\rangle = (1/\pi\hbar\omega)^{1/4} \times \exp[-(y-p)^2/2\hbar\omega - ixp/\hbar + ixy/2\hbar]. \tag{6}$$

With $z = 0$ ($x = 0, y = 0$), Eqs. (5) and (6) give the representations of coherent vector $|0\rangle$. Moreover, we have the well-known relation $|z\rangle = W(z)|0\rangle$, where $W(z)$ is the unitary (Weyl) operator

$$W(z) \equiv \exp(zZ^\dagger - z^*Z) = W(x,y) = \exp[i(yQ - xP)/\hbar]. \tag{7}$$

We say that a system is in a coherent state if and only if its (individual) state operator is

$$\rho = P_z \equiv |z\rangle\langle z| = \rho^2. \tag{8}$$

These pure states are minimum uncertainty in phase space ($\Delta Q \Delta P = \hbar/2$).

Several linear mappings from the set of self-adjoint operators A on $\mathscr{H}$ to the set of complex-valued functions on the classical phase space Ω have been considered in the literature.[7] In our physical context, these mappings are attempts to find a phase-space representation of an individual quantum system. We will consider only three important examples, namely, the Blokhintzev phase-space map[8]

$$r(q,p;A) \equiv 2\pi\hbar\langle q|A|p\rangle\langle p|q\rangle \tag{9a}$$
$$= \iint \frac{d\theta\, d\tau}{2\pi\hbar} e^{-i(\theta q + \tau p)/\hbar}\mathrm{Tr}(e^{i\theta Q/\hbar}Ae^{i\tau P/\hbar}), \tag{9b}$$

the Wigner phase-space map[9]

$$g(q,p;A) \equiv \iint \frac{d\theta\, d\tau}{2\pi\hbar} e^{-i(\theta q + \tau p)/\hbar}\mathrm{Tr}(Ae^{i(\theta Q + \tau P)/\hbar}) \tag{10a}$$
$$= \iint \frac{d\xi\, d\eta}{\pi\hbar} r(q+\xi, p+\eta; A)e^{2i\xi\eta/\hbar}, \tag{10b}$$

and the Wehrl phase-space map[1]

$$f(q,p;A) \equiv \langle q,p|A|q,p\rangle \tag{11a}$$
$$= \iint \frac{d\xi\, d\eta}{\sqrt{2}\pi\hbar} r(q+\xi, p+\eta; A)e^{i\xi\eta/\hbar}e^{-(\omega^2\xi^2+\eta^2)/2\hbar\omega}, \tag{11b}$$

where $|q,p\rangle$ is the coherent vector $|z\rangle$ with $x = q$ and $y = p$. The Blokhintzev and the Wigner maps are not real (i.e., $r^* \neq r$ and $g^* \neq g$), while the Wehrl map is real and nonnegative (i.e., $f^* = f \geqslant 0$). For every ρ and A, we have

$$\iint \frac{dq\, dp}{2\pi\hbar} r(q,p;\rho) = \iint \frac{dq\, dp}{2\pi\hbar} g(q,p;\rho) = \iint \frac{dq\, dp}{2\pi\hbar} f(q,p;\rho) = \mathrm{Tr}\,\rho = 1 \tag{12}$$

and

$$\iint \frac{dq\, dp}{2\pi\hbar} r^*(q,p;A)r(q,p;\rho) = \iint \frac{dq\, dp}{2\pi\hbar} g^*(q,p;A)g(q,p;\rho) = \mathrm{Tr}\,A\rho. \tag{13}$$

For the Wehrl map, instead, the relation

$$\iint \frac{dq\, dp}{2\pi\hbar} f(q,p;A)f(q,p;\rho) = \mathrm{Tr}\,A\rho \tag{14}$$

holds for every A only for the special class of (Wehrl) states ρ for which

$$\rho = \iint \frac{dq\, dp}{2\pi\hbar} f(q,p;\rho)|q,p\rangle\langle q,p|. \tag{15}$$

The usual interpretation of these relations is that the maps $r(q,p;\rho)$, $g(q,p;\rho)$, and $f(q,p;\rho)$ play a role analog to that of the classical phase-space state function, and the maps $r^*(q,p;A)$, $g^*(q,p;A)$, and $f(q,p;A)$ a role analog to that of the classical phase-space function associated with observable A. A discussion of the time evolution of $r(q,p;\rho)$ under Hamiltonian dynamics is given in Ref. 8.

III. CLASSICAL REPRESENTATION OF QUANTUM KINEMATICS

Ideally, a classical phase-space representation of a quantum system would be complete if it were possible to solve the following general problem. Given a system with quantum-mechanical Hilbert space $\mathscr{H}$ and classical-mechanical phase space Ω, find two mappings $w(q,p;\rho)$ and $a(q,p;A)$ that satisfy the following rather restrictive conditions. For every state operator ρ on $\mathscr{H}$, every well-defined self-adjoint operator A on $\mathscr{H}$, every point q,p in Ω, and every continuous real function $F(t)$ of the real variable t,

(i) $w(q,p;\rho)$ is real and nonnegative,

(ii) $a(q,p;A)$ is real,

(iii) $\displaystyle\iint \frac{dq\, dp}{2\pi\hbar} F(w(q,p;\rho)) = \mathrm{Tr}\,F(\rho)$,

(iv) $\displaystyle\iint \frac{dq\, dp}{2\pi\hbar} F(a(q,p;A))w(q,p;\rho) = \mathrm{Tr}\,F(A)\rho$.

Clearly, for $F(t) = -kt\ln t$ if $0 < t \leqslant 1$ and $F(t) = 0$ elsewhere, condition (iii) implies that $s^{\mathrm{cl}}(w) = s(\rho)$.

No rigorous solution to this problem is known. To the best of our knowledge, even the physically interesting question whether the problem admits of solutions, let alone to find them, remains unresolved. In what follows, we discuss the rudiments of an approach that may provide useful insight towards a resolution of the question.

IV. CLASSICAL LIMIT OF PHASE-SPACE FUNCTIONS

Let us consider the spectral expansion of the state operator

$$\rho = \sum_j w_j P_j, \tag{16}$$

$$I = \sum_j P_j, \tag{17}$$

$$P_j P_k = \delta_{jk} P_j, \tag{18}$$

where I is the identity and P_j the projector onto the eigenspace belonging to eigenvalue w_j, with degeneracy $d_j = \mathrm{Tr}\, P_j$. We readily verify that

$$\iint \frac{dq\, dp}{2\pi\hbar}\, r(q,p;P_j) = \mathrm{Tr}\, P_j = d_j, \tag{19}$$

$$\sum_j r(q,p;P_j) = 1, \tag{20}$$

$$r(q,p;\rho) = \sum_j w_j r(q,p;P_j), \tag{21}$$

and similar relations hold for the mappings g and f.

Using the relations

$$\iint \frac{d\xi\, d\eta}{2\pi\hbar}\, \xi^n \eta^m e^{i\xi\eta/\hbar} = \delta_{nm} i^n \hbar^n n!, \tag{22}$$

$$\iint \frac{d\xi\, d\eta}{\sqrt{2}\pi\hbar}\, \xi^n \eta^m e^{i\xi\eta/\hbar} e^{-(\omega^2\xi^2+\eta^2)/2\hbar\omega} = \begin{cases} 0 & \text{if } n+m \text{ odd}, \\ \dfrac{1\cdot 3\cdots(n+m-1)}{2^{n+m}} (\hbar\omega)^{m/2} (\hbar/\omega)^{n/2} & \text{if } n+m \text{ even}, \end{cases} \tag{23}$$

and the expansion

$$r(q+\xi, p+\eta; A) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{\partial^{n+m} r}{\partial q^n\, \partial p^m}\bigg|_{q,p;A} \frac{\xi^n \eta^m}{n!m!} \tag{24}$$

into Eqs. (10b) and (11b), we find

$$g(q,p;A) = r(q,p;A) + \sum_{n=1}^{\infty} \frac{\partial^{2n} r}{\partial q^n\, \partial p^n}\bigg|_{q,p;A} \frac{i^n \hbar^n}{n!}, \tag{25}$$

$$f(q,p;A) = r(q,p;A) + \sum_{n=1}^{\infty}\sum_{k=0}^{2n} \frac{\partial^{2n} r}{\partial q^k \partial p^{2n-k}}\bigg|_{q,p;A} \frac{1\cdot 3\cdots(2n-1)}{4^n}\, \omega^{n-k} \hbar^n, \tag{26}$$

and, after some manipulations involving Relations (18) and (22),

$$r(q,p;P_j) r(q,p;P_k) = \delta_{jk} r(q,p;P_j) - \sum_{n=1}^{\infty} \frac{(-i)^n \hbar^n}{n!} \frac{\partial^n r}{\partial q^n}\bigg|_{q,p;P_j} \frac{\partial^n r}{\partial p^n}\bigg|_{q,p;P_k}. \tag{27}$$

Relations (20) and (27) imply that the functions $r(q,p;P_j)$ have overlapping supports which cover the whole phase space Ω, i.e.,

$$\bigcup_j \Omega_j = \Omega, \tag{28}$$

$$\Omega_j \cap \Omega_k \neq \delta_{jk} \Omega_j, \tag{29}$$

where

$$\Omega_j \equiv \{q,p \,|\, r(q,p;P_j) \neq 0\}. \tag{30}$$

However, the relative importance of the overlap is small. For example, $|\int r_j r_k|^2 / |\int r_j^2| |\int r_k^2|$ is of order $\hbar^2/d_j d_k$ for $j \neq k$. Thus we conclude that, in the classical limit $\hbar \to 0$, the spectral expansion of the state operator ρ induces a partition of the phase-space Ω into disjoint cells Ω_j each belonging to a distinct eigenvalue w_j of ρ.

From Eqs. (25) and (26), it follows that if the Blokhintzev map $r(q,p;A)$, the Wigner map $g(q,p;A)$, and the Wehrl map $f(q,p;A)$ each admit of a classical limit as $\hbar \to 0$, then they tend to the same map. Assuming that such limits exist, we introduce the following notation

$$w(q,p) \equiv \lim_{\hbar\to 0} r(q,p;\rho) = \lim_{\hbar\to 0} g(q,p;\rho) = \lim_{\hbar\to 0} f(q,p;\rho), \tag{31}$$

$$a(q,p) \equiv \lim_{\hbar\to 0} r^*(q,p;A) = \lim_{\hbar\to 0} g^*(q,p;A) = \lim_{\hbar\to 0} f(q,p;A), \tag{32}$$

$$\alpha_j(q,p) \equiv \lim_{\hbar\to 0} r(q,p;P_j) = \lim_{\hbar\to 0} g(q,p;P_j) = \lim_{\hbar\to 0} f(q,p;P_j). \tag{33}$$

It then follows from Relations (20), (21), and (27) that

$$\sum_j \alpha_j(q,p) = 1, \tag{34}$$

$$w(q,p) = \sum_j w_j \alpha_j(q,p), \tag{35}$$

$$\alpha_j(q,p)\alpha_k(q,p) = \delta_{jk}\alpha_j(q,p), \tag{36}$$

and, therefore, the functions $\alpha_j(q,p)$ can only take the values 0 and 1, and have nonoverlapping supports covering the whole phase space. Thus the structure of the function w is such that

$$F(w(q,p)) = \sum_j F(w_j)\alpha_j(q,p) \tag{37}$$

in analogy with the general relation

$$F(\rho) = \sum_j F(w_j) P_j. \tag{38}$$

To proceed further, we conjecture that

$$\iint \frac{dq\, dp}{2\pi\hbar}\, \alpha_j(q,p) = d_j. \tag{39}$$

We have no proof for this. The conjecture is based only on some heuristic arguments. We first note that Relation (39) is consistent with the improper formal relations

$$\iint \frac{dq\, dp}{2\pi\hbar}\, 1 = \iint \frac{dq\, dp}{2\pi\hbar}\, r(q,p;I) = \mathrm{Tr}\, I = \sum_j d_j, \tag{40}$$

$$\iint \frac{dq\,dp}{2\pi\hbar} 1 = \iint \frac{dq\,dp}{2\pi\hbar} \sum_j \alpha_j(q,p)$$

$$= \sum_j \iint \frac{dq\,dp}{2\pi\hbar} \alpha_j(q,p), \quad (41)$$

where we used that fact that $r(q,p;I) = 1$ and Relation (34). Moreover, we note that it is consistent with the requirement that if $w(q,p)$ is to represent a classical state function, then it must be normalized and, therefore,

$$\iint \frac{dq\,dp}{2\pi\hbar} w(q,p) = \sum_j w_j \iint \frac{dq\,dp}{2\pi\hbar} \alpha_j(q,p)$$

$$= 1 = \sum_j w_j d_j. \quad (42)$$

Finally, we observe that the conjecture and the normalization condition for $w(q,p)$ would follow if there were a meaning to saying that the phase-space measure $dq\,dp/2\pi\hbar$ is independent of $\hbar$ so that the following relation would make sense at least for A in the trace class

$$\operatorname{Tr} A = \iint \frac{dq\,dp}{2\pi\hbar} r(q,p;A) = \lim_{\hbar\to 0} \iint \frac{dq\,dp}{2\pi\hbar} r(q,p;A)$$

$$= \iint \frac{dq\,dp}{2\pi\hbar} \lim_{\hbar\to 0} r(q,p;A). \quad (43)$$

If the conjecture could be proved, then from Relations (37) and (38) it would follow that

$$\iint \frac{dq\,dp}{2\pi\hbar} F(w(q,p)) = \iint \frac{dq\,dp}{2\pi\hbar} \sum_j F(w_j)\alpha_j(q,p)$$

$$= \sum_j F(w_j) d_j = \operatorname{Tr} F(\rho), \quad (44)$$

which would prove that the function $w(q,p)$ [Relation (31)] satisfies conditions (i) and (iii) of Sec. III and that, in particular, $s^{\rm cl}(w) = s(\rho)$. In a similar manner, and with similar conjectures, we would show that the function $a(q,p)$ [Relation (32)] satisfies conditions (ii) and (iv).

Because it is not clear whether Relations (39)–(43) admit of a rigorous justification, we conclude that the question of existence of solutions to the problem defined in Sec. III remains unresolved.

V. CONCLUSIONS

We have given restrictive conditions defining a complete classical phase-space representation of quantum kinematics for systems with both a classical and a quantum description. Whether such representations exist is an unresolved problem. We presented heuristic arguments in support of the usual unproved claim that $s(\rho)\to s^{\rm cl}(w)$ in the classical limit $\hbar\to 0$.

We have observed that, in the limit $\hbar\to 0$, the spectral expansion of the quantum state operator ρ induces a partition of the phase space Ω into disjoint cells Ω_j each belonging to a distinct eigenvalue w_j of ρ. Over cell Ω_j, the classical state function w has the constant value w_j. We conjectured that the phase-space volume of cell Ω_j equals the degeneracy d_j of eigenvalue w_j. Accordingly, the phase-space volume of the support of w, i.e., of the complement of cell Ω_0 belonging to the zero eigenvalue of ρ, cannot be smaller than the value 1 attained for every idempotent or pure state ($\rho^2 = \rho$).

We conclude with a remark on dynamics, namely, on the distinction between conservation of volume in phase space and thermodynamic reversibility. It is true that the Liouville–von Neumann equation for the unitary evolution of ρ induces in the classical limit an evolution of w which preserves both the volume of the support of w and the value of the entropy. However, it is seldom recognized explicitly that conservation of volume in phase space is not equivalent to thermodynamic reversibility. For example, we could conceive of nonunitary evolution equations which preserve the volume of the support of w (i.e., equations that preserve the zero eigenvalues of ρ) but not the value of the entropy (i.e., such that the nonzero eigenvalues of ρ are not invariant). We believe[3] this to be an interesting and physically important feature of a recently proposed[10] nonlinear quantum equation of motion for a single elementary constituent of matter.

ACKNOWLEDGMENT

The author gratefully acknowledges financial support of the Thermo Electron Corporation.

[1]A. Wehrl, Rep. Math. Phys. **16**, 353 (1979). See also A. Wehrl, Rev. Mod. Phys. **50**, 221 (1978) and E. H. Lieb, Commun. Math. Phys. **62**, 35 (1978).

[2]G. N. Hatsopoulos and E. P. Gyftopoulos, Found. Phys. **6**, 15, 127, 439, 561 (1976).

[3]G. P. Beretta, E. P.Gyftopoulos, J. L. Park, and G. N. Hatsopoulos (in press).

[4]A most instructive essay on the conceptual problems arising from the traditional use of the statistical operator is found in J. L. Park, Am. J. Phys. **36**, 211 (1968).

[5]A most persuasive proof that the entropy of any system (even a single particle) in any state ρ (equilibrium and nonequilibrium) is $s(\rho) = -k \operatorname{Tr} \rho \ln \rho$ is given in Ref. 2.

[6]See, e.g., J. R. Klauder and E. C. G. Sudarshan, *Fundamentals of Quantum Optics* (Benjamin, New York, 1968), Chap. 7.

[7]L. Cohen, J. Math. Phys. **7**, 781 (1966); L. Cohen, in *Contemporary Research in the Foundations and Philosophy of Quantum Theory*, edited by C. A. Hooker (Dordrecht, Holland, 1973), p. 66; J. L. Park, W. Band, and W. Yourgrau, Ann. Phys. **7.37**, 189 (1980) and references therein.

[8]D. I. Blokhintzev, J. Phys. **2**, 71 (1940); D. I. Blokhintzev and P. Nemirovsky, J. Phys. **3**, 291 (1940).

[9]E. Wigner, Phys. Rev. **40**, 749 (1932).

[10]G. P. Beretta, Thesis, (MIT, 1981) (unpublished). The new equation for a single elementary constituent of matter is presented in Ref. 3.