On the classical limit of phasespace formulation of quantum mechanics: Entropy

Lipo Wang

Citation: Journal of Mathematical Physics 27, 483 (1986); doi: 10.1063/1.527247

View online: http://dx.doi.org/10.1063/1.527247

View Table of Contents: http://scitation.aip.org/content/aip/journal/jmp/27/2?ver=pdfcov

Published by the AIP Publishing
On the classical limit of phase-space formulation of quantum mechanics: Entropy

Lipo Wang
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

(Received 30 May 1985; accepted for publication 9 September 1985)

The classical limits of phase-space formulation of quantum mechanics are studied. As a special example, some properties of both quantum mechanical and classical entropies are discussed in detail.

I. INTRODUCTION

It has been common knowledge that quantum mechanics approaches classical mechanics when Planck's constant approaches zero. Rigorous investigations have been carried out during the last decade by various authors. So far the methods employed are restricted to the quantum mechanical operator techniques and the questions considered are mainly partition function and ensemble average. The purpose of the present work is to examine the general problem of the classical limit $\hbar \to 0$ by means of the so-called phase-space formalism of quantum mechanics. With the help of the general results, the unsolved problem of the behavior of quantum mechanical entropies at the classical limit is discussed.

The phase-space formulation of quantum mechanics has found many applications, particularly in statistical mechanics and quantum optics. Its basic feature is to provide a framework for the treatment of quantum mechanical problems in terms of classical concepts. Following the appearance of the well-known Wigner distribution function, many other distribution functions have been considered. For instance, the antinormal-ordered (Husimi) and the normal-ordered (P) distribution functions, the anti-standard-ordered (Kirkwood) and the standard-ordered distribution functions. Each of those distribution functions was created for a particular purpose.

Considering the properties of entropies, Wehrl stated, "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 a recent paper, Beretta took the first attempt at this question. But some weak points can be found in Beretta's investigation, as shown in our paper. In fact, both quantum mechanical and classical entropies are singular at the classical limit, however, the difference between them does vanish at this limit.

The paper is organized as follows. In Sec. II we briefly review the concepts of the phase-space formalism of quantum mechanics. Some useful results are derived. In Sec. III the classical limit of quantum mechanical description is considered. We discuss the relation between quantum mechanical and classical entropies in Sec. IV. Conclusions and discussions are presented in Sec. V. Also, in the Appendix, we wish to make some comments on the problems of complete classical phase-space representation of quantum kinematics and spectral expansion in the classical limit $\hbar \to 0$ discussed in Ref. 12.

We are going to restrict our discussion to the case of one degree of freedom so that the Hilbert space is $\mathcal{H} = L^2(R)$ and phase space is $\mathcal{P} = R^2$. But we wish to emphasize that the arguments can be easily extended to the case of many degrees of freedom.

II. THE GENERAL CLASSICAL PHASE-SPACE REPRESENTATION OF QUANTUM MECHANICAL OPERATORS

The mathematical form of the general question about the classical phase-space representation of quantum mechanical operators is stated as follows. Suppose $A$ and $B$ are two Hermitian operators. Find a pair of mappings, $\Theta$ and $\Theta'$, say, on phase space, which have the following properties:

$$\Theta(A) = a(q, p),$$

$$\Theta'(B) = b'(q, p),$$

and

$$\text{Tr}(\hat{A}) = \int \int a(q, p) dq dp,$$

$$\text{Tr}(\hat{A}\hat{B}) = \int \int a(q, p)b'(q, p) dq dp.$$
The inversion is
\[ a(q, p) = \text{Tr}(\hat{\Delta}^{(\Delta)}(q - \hat{q}, p - \hat{p})) \]  
(10)
Each mapping is characterized by a so-called filter function \( \Omega(u, v) \) (Table I), which is chosen to satisfy the trivial normalization condition
\[ \Omega(0, 0) = 1. \]  
(11)
The operator \( \Delta^{(\Delta)}(q - \hat{q}, p - \hat{p}) \) is defined in the same fashion as Eq. (9) with filter function
\[ \hat{\Omega}(u, v) = |\Omega(-u, -v)|^{-1}. \]  
(12)
The problem of expressing an operator in an ordered form according to a prescribed rule is equivalent to an appropriate mapping of the operator on phase space.

The second mapping \( \Omega' \) is determined by
\[ \hat{\Omega}' = \int b'(q, p) \Delta^{(\Delta)}(q - \hat{q}, p - \hat{p}) dq dp, \]  
(13)
with inversion
\[ b'(q, p) = 2\pi \hbar \text{Tr}(\hat{\Delta}^{(\Delta)}(q - \hat{q}, p - \hat{p})). \]  
(14)
It is clear that
\[ \Theta = (2\pi \hbar)^{-1} \Theta'. \]  
(15)
Next we wish to find the relation between two different mappings \( \Omega_1 \) and \( \Omega_2 \) say. The \( \Delta \)-operator can be expressed in a slightly different form
\[ \Delta^{(\Delta)}(q - \hat{q}, p - \hat{p}) = (2\pi \hbar)^{-2} \int \Omega_j(u, v) \hat{D}(u, v) \exp \left( -i \frac{qu + pv}{\hbar} \right) du dv, \]  
(16)
where \( j = 1, 2 \),
\[ \hat{D}(u, v) = \exp(iu\hat{q} + vp)/\hbar \]  
(17)
is the well-known displacement operator if we define
\[ \hat{q} = (2\hbar)^{-1/2}(\hat{q} + i\hat{p}), \]  
(18)
and
\[ \alpha = (2\hbar)^{-1/2}(-u + iv). \]  
(19)
We observe that
\[ \Delta^{(\Delta)}(q - \hat{q}, p - \hat{p}) = (2\pi \hbar)^{-2} \int \left( \frac{\Omega_j(u, v)}{\Omega_1(u, v)} \right) \Omega_1(u, v) \hat{D}(u, v) \times \exp \left( -i \frac{qu + pv}{\hbar} \right) du dv \]  
(20)
\[ \times \Delta^{(\Delta)}(\hat{q} - \hat{p}, \hat{p} - \hat{q}). \]  
From Eqs. (10) and (20) it follows that
\[ a^{(\Delta)}(q, p) = L_{21} \left( -i\frac{\partial}{\partial q}, -i\frac{\partial}{\partial p} \right) a^{(\Delta)}(q, p), \]  
(21)
where
\[ L_{21}(x, y) = \Omega_2(x, y)/\Omega_1(x, y). \]  
(22)
Letting \( \hat{\Omega}_j \rightarrow \Omega_j, j = 1, 2 \), and using Eq. (9), we obtain the following differential relation between \( a^{(\Delta)}(q, p) \) and \( a^{(\Delta)}(q, p) \):
\[ a^{(\Delta)}(q, p) = L_{12} \left( -i\frac{\partial}{\partial q}, -i\frac{\partial}{\partial p} \right) a^{(\Delta)}(q, p). \]  
(23)
In particular, we choose \( \hat{\lambda} = \hat{p} \), which is the density operator describing the system of interest, then \( a(q, p) \) serves as if it were a classical distribution function. Conventionally \( b'(q, p) \) defined by Eq. (13) is called the \( \Omega \)-equivalence of operator \( \hat{B} \) and \( a(q, p) \) defined by Eq. (10) the \( \Omega \)-distribution function, which is usually denoted by \( P^{(\Omega)}(q, p) \). Thus the expectation value of a quantum mechanical observable \( \hat{B} \) can be written in a classical form
\[ \langle \hat{B} \rangle = \text{Tr}(\hat{p}\hat{B}) = \int b''(q, p) P^{(\Omega)}(q, p) dq dp. \]  
(24)
Also the distribution thus defined satisfies the normalization condition
\[ \int P^{(\Omega)}(q, p) dq dp = \text{Tr}(\hat{\rho}) = 1. \]  
(25)
For example, if we consider the simplest case where \( \hat{\Omega}(u, v) = \Omega(u, v) = 1 \), then it leads to the famous Wigner distribution function and the Wigner equivalence (denoted by suffix \( \omega \)):
\[ b^{(\omega)}(q, p) = \int \left( p - \frac{u}{2} \right)^2 |\hat{B}|^2 + \frac{u}{2} \exp \left( -i\frac{qu}{\hbar} \right) du, \]  
(27)
The Wigner equivalence of an operator \( \hat{F} = \hat{B}\hat{C} \) can be expressed in terms of those corresponding to \( \hat{B} \) and \( \hat{C} \) through the Groenewold theorem,\(^{13}\)
\[ f^{(\omega)}(q, p) = b^{(\omega)}(q, p) \exp(\hbar\hat{G}/2i) c^{(\omega)}(q, p), \]  
(28)
where
\[ \hat{G} = \left( \frac{\partial}{\partial p} \right) \left( \frac{\partial}{\partial q} \right) - \left( \frac{\partial}{\partial q} \right) \left( \frac{\partial}{\partial p} \right), \]  
(29)
and the arrows indicate in which direction the derivatives act.

One of the major advantages of the Wigner equivalence is that it leads to the simplest forms for the quantum corrections to the corresponding classical quantity,\(^{14}\) and therefore is very useful to the semiclassical calculations.\(^{15}\) It can assume negative values, which makes it quite different from classical distribution functions.

Another choice of the filter function leads to the antistandard-ordered distribution function\(^6\) (see Table I),

<table>
<thead>
<tr>
<th>Rule of association</th>
<th>( \Omega(u, v) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weyl</td>
<td>( p^n q^m \rightarrow (\hat{q}^n \hat{p}^m) )</td>
</tr>
<tr>
<td>Standard</td>
<td>( p^n q^m \rightarrow \hat{q}^n \hat{p}^m ) ( \exp(-iuv/2\hbar) )</td>
</tr>
<tr>
<td>Antistandard</td>
<td>( p^n q^m \rightarrow \hat{p}^n \hat{q}^m ) ( \exp(iuv/2\hbar) )</td>
</tr>
</tbody>
</table>

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 155.69.5.71 On: Sun, 05 Jan 2014 13:56:00
which has the important property that it is non-negative everywhere in phase space. The class of non-negative quantum distribution functions has been shown to be rather small.17

III. CLASSICAL LIMIT $\hbar \to 0$

With the help of the formulas mentioned in the Sec. II, we now consider taking the classical limit $\hbar \to 0$.

First of all we observe from Eqs. (11), (22), and (23) that any phase-space distribution function that describes the same system, approaches the same limit at $\hbar \to 0$. Also, any phase-space equivalence (resulting from any rule of association) of the same quantum mechanical operator approaches the same limit at $\hbar \to 0$. Explicitly we have

$$\lim_{\hbar \to 0} b^{(n)}(q, p) = b^{(\text{cl})}(q, p), \quad (30)$$

and

$$\lim_{\hbar \to 0} P^{(n)}(q, p) = P^{(\text{cl})}(q, p). \quad (31)$$

Of course the necessary and sufficient condition for any of Eqs. (30) and (31) to be true is that the appropriate limit exists, which will be assumed in the following discussion.

Equation (31) thus defines a classical distribution, $P^{(\text{cl})}(q, p)$. We can prove that $P^{(\text{cl})}(q, p)$ is real and non-negative everywhere in phase space simply by choosing a real and non-negative quantum distribution function, e.g., the anti-standard-ordered distribution function, on the left-hand side of Eq. (31). In the case of a canonical ensemble, $P^{(\text{cl})}(q, p)$ turns out to be the Maxwell–Boltzmann distribution.5

Now we would like to consider the properties that the “classical functions” $b^{(\text{cl})}(q, p)$ and $P^{(\text{cl})}(q, p)$ possess. The conclusions at which we just arrived make it enough to restrict ourselves within the Wigner equivalence and distribution function.

By using Eqs. (28) and (29) we get the Wigner equivalence and distribution function.

$$\langle \hat{B}^n \rangle' = b^{(n)}(q, p) \exp(iH\omega/2\hbar) \langle \hat{B}^n-1 \rangle'$$

$$= b^{(n)}(q, p) \exp(iH\omega/2\hbar)$$

$$\times \left[ b^{(n)}(q, p) \exp(iH\omega/2\hbar) \langle \hat{B}^{n-2} \rangle' \right]. \quad (32)$$

Obviously, $\exp(iH\omega/2\hbar)$ approaches its identity at $\hbar \to 0$.

Hence

$$\lim_{\hbar \to 0} \langle \hat{B}^n \rangle' = (b^{(\text{cl})}(q, p))^n. \quad (33)$$

It is easy to see that for any infinitely differentiable function $R(t)$, we have the following useful relation:

$$\lim_{\hbar \to 0} \langle \hat{R}(\hat{B}) \rangle' = R(b^{(\text{cl})}(q, p)), \quad (34)$$

where suffix $\Omega$ denotes an arbitrary $\Omega$-equivalence.

On the other hand we have

$$\text{Tr}(\hat{R}(\hat{B})) = \langle \int P^{(\text{cl})}(q, p)\langle R(\hat{B}) \rangle' dq dp \rangle. \quad (35)$$

Let $\hbar \to 0$ at both sides

$$\lim_{\hbar \to 0} \langle \hat{R}(\hat{B}) \rangle' = (\langle \hat{R}(\hat{B}) \rangle)'_\text{cl}, \quad (36)$$

where

$$\langle \hat{R}(\hat{B}) \rangle' = \int P^{(\text{cl})}(q, p)\langle R(b^{(\text{cl})}(q, p)) dq dp, \quad (37)$$

and its existence has been assumed.

IV. RELATION BETWEEN QUANTUM MECHANICAL AND CLASSICAL ENTROPY

Traditionally entropy is introduced in the phenomenological thermodynamical considerations based on the second law of thermodynamics. The conception of entropy thus defined frequently leads to some obscure ideals.18 The well-known heat death provides a good example. In classical statistical mechanics the Boltzmann and the Gibbs entropies are not very good ones either. The reason is that they never lead to the third law of thermodynamics. Thus a correct definition of entropy is only possible in the framework of quantum mechanics.

If a system is described by a density operator $\hat{\rho}$, its entropy is then defined quantum mechanically by

$$S(\hat{\rho}) = -k \text{Tr}(\hat{\rho} \ln \hat{\rho})$$

$$= -k \int P^{(\text{cl})}(q, p)\ln P^{(\text{cl})}(q, p) dq dp$$

$$= -k \int P^{(\text{cl})}(q, p)\{\ln \left(\frac{\hat{\rho}}{2\pi \hbar} \right)^{\text{cl}}\} dq dp - k \ln(2\pi \hbar). \quad (38)$$

Noticing that

$$\langle \hat{\rho}/2\pi \hbar \rangle^\text{cl} = P^{(\text{cl})}(q, p), \quad (39)$$

we find, according to Eq. (36), that the first term in Eq. (38) approaches

$$-k \int P^{(\text{cl})}(q, p)\ln P^{(\text{cl})}(q, p) dq dp \quad (40)$$

in the limit $\hbar \to 0$. But the second term diverges to positive infinity. If the classical entropy functional is defined by

$$S^{(\text{cl})}(P^{(\text{cl})}) = -k \int P^{(\text{cl})}(q, p)\ln P^{(\text{cl})}(q, p) dq dp - k \ln(2\pi \hbar),$$

(41)

then the quantum mechanical entropy approaches the classical entropy functional in the limit $\hbar \to 0$, in the following sense:

$$\lim_{\hbar \to 0} \{S(\hat{\rho}) - \ln(2\pi \hbar)\} = \lim_{\hbar \to 0} \{S^{(\text{cl})}(P^{(\text{cl})}) - \ln(2\pi \hbar)\} = 0. \quad (42)$$

or

$$\lim_{\hbar \to 0} \{S(\hat{\rho}) - S^{(\text{cl})}(P^{(\text{cl})})\} = 0. \quad (43)$$

Let us consider a simple example, i.e., an ensemble of harmonic oscillators with a heat bath of temperature $T$. The easiest way to compute the quantum mechanical entropy is to use the Wigner phase-space equivalence and distribution function.

From Ref. 20,

$$b^{(r)}(q, p) = (\exp(-\beta \hbar))^a$$

$$\text{sech}(\hbar \omega \beta/2)\exp(-2 \tanh(\hbar \omega \beta/2)(H/\hbar \omega)), \quad (44)$$
and the partition function is
\[ Z = \text{Tr}(\exp(-\beta \hat{H})) \]
\[ = (2\pi\hbar)^{-1} \int b^{*}(q, p) b dq dp \]
\[ = (2 \sinh(\hbar \beta / 2))^{-1}. \tag{45} \]

Hence the Wigner distribution function is an immediate result of Eqs. (44) and (45),
\[ P^{(w)}(q, p) = (\beta / 2\pi\hbar)^{1/2} \]
\[ = b^{*}(q, p)/(2\pi\hbar Z) \]
\[ = (\pi\hbar)^{-1} \tan(\hbar \beta / 2) \]
\[ \times \exp(-2/\hbar \beta \tan(\hbar \beta / 2) \hat{H}), \tag{46} \]

where the Hamiltonian is
\[ \hat{H} = \hat{p}^2/2m + \hbar \omega \hat{q}^2/2. \tag{47} \]

The quantum mechanical entropy can be obtained by
\[ S(\hat{p}) = k \left( \ln Z - \beta \frac{\partial \ln Z}{\partial \beta} \right) \]
\[ = (k\beta \hbar \omega /2) \tan(\hbar \beta /2) \]
\[ - k \ln(2 \sinh(\hbar \beta /2)). \tag{48} \]

The Wigner distribution function approaches the classical canonical distribution function at \( \hbar \to 0, \)
\[ \lim_{\hbar \to 0} P^{(w)}(q, p) = (\omega \beta /2\pi)\exp(-\beta H), \tag{49} \]
as predicted by the general considerations. The classical partition function is, by definition,
\[ Z^{(c)} = (\hbar \omega \beta)^{-1}. \tag{50} \]

Finally, the classical entropy has the form
\[ S^{(c)} = k - k \ln(\hbar \omega \beta). \tag{51} \]

With the help of Eqs. (48) and (51), Eqs. (42) and (43) are maintained.

V. CONCLUSIONS

We discussed the general phase-space representation of quantum mechanics at the classical limit \( \hbar \to 0. \) We proved that every representation approaches the same "limit representation" at \( \hbar \to 0. \) The open question on the relation between the classical and quantum mechanical entropies was answered. The differences between the classical and quantal entropies are shown to approach zero at the classical limit \( \hbar \to 0. \)

ACKNOWLEDGMENTS

The author wishes to thank Professor R. F. O'Connell for many helpful conversations.

This research was partially supported by the Division of Materials Science, U. S. Department of Energy under Grant No. DE-FG05-84ER45135.

APPENDIX: COMMENTS ON TWO OF THE PROBLEMS DISCUSSED IN REF. 12

In a recent paper, Beretta gave a set of rather restrictive conditions defining a complete classical phase space representation of quantum kinematics for systems with both classical and quantum mechanical descriptions. With help of the general considerations of phase-space representation we wish to make some comments on Beretta's ideals and derivations. In order to keep consistent with the notions that we have been using, we quote those conditions in a slightly different form.

Given a system with quantum mechanical Hilbert space \( \mathcal{H} \) and classical space \( \mathcal{P}, \) find two mappings \( w(q, p; \hat{p}) \) and \( b(q, p; \hat{B}) \) that satisfy the following conditions. For every density operator \( \hat{\rho} \) on \( \mathcal{H}, \) every well-defined Hermitian operator \( \hat{B} \) on \( \mathcal{H}, \) every point \( (q, p) \) in \( \mathcal{P}, \) and every continuous real function \( R(t) \) of the real variable \( t, \)
1. \( w(q, p; \hat{p}) \) is real and non-negative,
2. \( b(q, p; \hat{B}) \) is real,
3. \( \int \int R(w(q, p; \hat{p})) dq dp = \text{Tr}(R(\hat{\rho})), \)
4. \( \int \int w(q, p; \hat{p}) R(b(q, p; \hat{B})) dq dp = \text{Tr}(\hat{\rho} R(\hat{B})). \)

(4) The purpose of seeking this representation is to show that the quantum mechanical entropy is exactly equal to a "classical entropy functional," which is defined by
\[ S^{(c)}(w) = - k \int \int w(q, p; \hat{p}) \ln 2\pi \hbar \omega w(q, p; \hat{p}) dq dp. \tag{5} \]

If such a representation exists, then we choose \( R(t) = - k \ln t \) and from (4.1) obtain
\[ S(\hat{p}) = - k T(\hat{p} \ln \hat{p}) = S^{(c)}(w). \tag{6} \]

Beretta did not know whether this representation existed or not. After making a conjecture, Beretta tried to prove that this representation was just the one to which the Wigner, the Blokhistev, and the Wehrl phase-space representations \( (R_o) \) converge in the classical limit \( \hbar \to 0. \)

Although we do not know whether this representation exists, we are able to conclude that \( R_o \) is an incorrect candidate for the representation, the reason being that in \( R_o, \) Eqs. (3) and (4) hold only after limit \( \hbar \to 0 \) are taken in the right-hand sides.

Now we turn to consider another problem discussed in Ref. 12: the behavior of the spectral expansions in the classical limit \( \hbar \to 0. \) The density operator can be written as follows:
\[ \hat{\rho} = \sum_{i=0}^{\infty} w_i \hat{\rho}_j, \tag{7} \]
where \( \hat{\rho}_j = |\psi_j \rangle \langle \psi_j | \) is the projector onto the eigenspace \( |\psi_j \rangle \) with eigenvalue
\[ \omega_j = [\exp(-\beta E_j)] / Z \tag{8} \]
and
\[ \hat{H} |\psi_j \rangle = E_j |\psi_j \rangle. \tag{8'} \]

By definition we have
\[ \sum_{j=0}^{\infty} \hat{\rho}_j = I, \tag{9} \]
where \( I \) denotes the identity operator.

The Wigner equivalences of Eqs. (7) and (8) are
The relation between $P^{(u)}(q, p)$ and $r(q, p; \hat{P}_j)$ in Ref. 12 is

$$P^{(u)}(q, p) = \sum_{j=0}^{\infty} w_j P_j^{(u)}(q, p). \quad (A10)$$

Next we consider letting $\hbar \to 0$. It has been shown that

$$\lim_{\hbar \to 0} P_j^{(u)}(q, p) = \delta(I(q, p) - I_j)/2\pi, \quad (A12)$$

where $I_j$ is the semiclassical action associated with $|\psi_j\rangle$ [i.e., $I_j = (j + \gamma\hbar)$ with $\gamma$ the Maslov index].

While quantization disappears in the classical limit $\hbar \to 0$, we expect

$$\lim_{\hbar \to 0} w_j = 0, \quad (A13)$$

since $w_j$ is the probability of the system being in state $|\psi_j\rangle$.

Thus when $\lim_{\hbar \to 0}$ is applied to both sides of Eq. (A10), the order of $\lim_{\hbar \to 0}$ and $\sum_{n=0}^{\infty}$ cannot be exchanged. Furthermore it is easily verified that

$$\sigma_j(q, p) = \lim_{\hbar \to 0} r(q, p; \hat{P}_j) = 0. \quad (A14)$$

Therefore Eqs. (34), (35), and (39), the conjecture, in Ref. 12 are not valid.

References:

10. See the recent reviews, e.g., R. F. O’Connell, Found. Phys. 13, 83 (1983);
19. For recent reviews see, e.g., A. Wehrl, Rev. Mod. Phys. 50, 221 (1978).
21. It is worth noticing that the Wehrl phase-space representation that Beretta referred to is actually the antinormal-ordered (Husimi) one. See, e.g., Ref. 6 and Ref. 7.