

Quantum Statistical Mechanics on Stochastic Phase Space¹

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Received: 18 August 1977

Abstract

Within the context of the theory of stochastic phase spaces, introduced in some earlier papers, a systematic mathematical procedure is developed for expressing quantum mechanical observables as generalized functions on a stochastic phase space. The states in such a theory are normalized, positive semidefinite, continuous functions of the phase space variables, satisfying marginality conditions appropriate to the stochastic nature of the underlying phase space. The action of a general quantum mechanical observable on the state space is then shown to lead in general to formal differential operators of finite or infinite order. Explicit computations of some typical operators are made to illustrate the theory. As a useful practical application, the theory is employed to derive a Bloch equation from which the Husimi transform of the canonical equilibrium state is then computed, after expressing it as an infinite series in powers of \hbar .

1. Introduction

The procedure for calibrating any given measuring apparatus \mathcal{A} is intrinsically stochastic in nature, since it involves repeated comparisons between the readings of that particular apparatus \mathcal{A} and another apparatus \mathcal{A}_0 , which is either chosen as a standard (such as the standard meter) or which has already been calibrated. Thus, no outcome of the measurement of any single observable A is ever exhaustively describable by a single number α , but rather a probability measure μ_α has to be included in the description. This measure embodies the calibrating procedure in the following way: If I denotes any interval (or, more generally, Borel set) on the real line, $\mu_\alpha(I)$ is a measure of the confidence that when the reading α is obtained with \mathcal{A} , the “actual value” of A was within I —i.e., roughly speaking, if a totally random set of infinitely precise values of A has been prepared by using the standard \mathcal{A}_0 , then the probability of obtaining with \mathcal{A} a reading α equals $\mu_\alpha(I)$ when the prepared

¹ Supported in part by a research grant from the National Research Council of Canada.

value falls within I . (Naturally, the term “infinitely precise” warrants a careful operational definition—cf. Prugovečki, 1976b, Appendix, and the references quoted therein.) We shall call the pair (α, μ_α) a *stochastic point* on the real line, and we shall say that $\hat{\alpha} = (\alpha, \mu_\alpha)$ is *sharp* if $\mu_\alpha(\{\alpha\}) = 1$, and that otherwise it is *nonsharp* or *fuzzy*.

Let us note that conceptually a stochastic point $\hat{\alpha}$ is distinct from a “value” α even in the case when $\hat{\alpha}$ is sharp, since even then it is the outcome of an intrinsically stochastic calibrating procedure, and the probabilistic statement that “the value α has been measured with a 100% confidence margin” is distinct from the categorical statement that “the system has the value α .” In this context, it is interesting to note that in principle a sharp stochastic point $\hat{\alpha}$ can be obtained only if α is an isolated value in the point spectrum of the observable A , but that this is a necessary and not a sufficient condition. For example, no actual measurement of a spin component is ever totally sharp, but can only be made “very nearly” sharp (cf. Prugovečki, 1977).

The above terminology is of little consequence, however, as long as a single observable A is measured, and as long as it is believed that *arbitrarily precise* measurements can be performed in principle. Indeed, the nonsharpness of actual measurements is usually taken into account by standard reduction-of-data procedures, routinely applied before inserting the raw experimental results into any given theoretical framework. Furthermore, if $\rho(\lambda)$ is any given probability distribution of sharp values of A , then the probability distribution $\hat{\rho}(\alpha)$ corresponding to the stochastic points $\hat{\alpha}$ is easily seen to be (Ali and Emch, 1974; Prugovečki, 1976a)

$$\hat{\rho}(\alpha) = \int_{\mathbb{R}^1} \rho(\lambda) \mu_\alpha(d\lambda) \quad (1.1)$$

However, this situation changes drastically as soon as for some given observable A there is reason to believe that there is a fundamental (and not just experimental) upper limit to the accuracy with which A can be measured (e.g., if there turns out to be a fundamental limit in the measurements of position of elementary particles), or if two or more incompatible observables are measured simultaneously. In that case, there can exist probability measures on sample spaces of fuzzy stochastic points that are not derivable from conventional probability measures on spaces of sharp sample points, as was the case in (1.1) (cf. Prugovečki, 1976a).

A notable example of a class of measures that are not derivable from measures on spaces of sharp sample points are those corresponding to the probability densities $\rho_g(q, p)$ (cf. Ali and Prugovečki, 1977a, b),

$$\rho_g(q, p) = h^{-N} \text{Tr}[U(q, p)gU^*(q, p)\rho] \quad (1.2)$$

$$U(q, p) = \exp\left(\frac{i}{\hbar} p \cdot Q\right) \exp\left(-\frac{i}{\hbar} q \cdot P\right) \quad (1.3)$$

$$p \cdot Q = p_1 Q_1 + p_2 Q_2 + \cdots + p_N Q_N, \quad q \cdot P = q_1 P_1 + q_2 P_2 + \cdots + q_N P_N \quad (1.4)$$

assigned to every density operator ρ describing the state of a spinless, non-relativistic quantum system with N degrees of freedom. In this context the generator g of the phase space representation is a positive operator of trace 1 which determines the confidence measures of the stochastic phase point (\hat{q}, \hat{p}) ,

$$\hat{q} = (q, \mu_q^{(g)}), \quad \mu_q^{(g)}(dq') = \chi_q^{(g)}(q') dq' \quad (1.5a)$$

$$\hat{p} = (p, \nu_p^{(g)}), \quad \nu_p^{(g)}(dp') = \chi_p^{(g)'}(p') dp' \quad (1.5b)$$

by determining the confidence functions $\chi_q^{(g)}$ and $\chi_p^{(g)'}$ of \hat{q} and \hat{p} , respectively (Prugovečki, 1976a), as follows:

$$\chi_q^{(g)}(q') = \chi_0^{(g)}(q' - q), \quad \chi_0^{(g)}(q') = \langle q' | g | q' \rangle \quad (1.6a)$$

$$\chi_p^{(g)'}(p') = \chi_0^{(g)'}(p' - p), \quad \chi_0^{(g)'}(p') = \langle p' | g | p' \rangle \quad (1.6b)$$

Thus, $\rho_g(q, p)$ is interpreted (Prugovečki, 1976a, b; Ali and Prugovečki, 1977a) as the probability density of obtaining the stochastic points \hat{q} and \hat{p} as outcomes of the simultaneous measurement of the position and momentum observables Q and P on an ensemble in the state ρ (concrete measurement procedures of this kind are discussed in Prugovečki, 1976b). As might be expected, $\rho_g(q, p)$ is not derivable from a probability distribution at sharp phase space points (Ali and Prugovečki, 1977a); however, it satisfies the following marginality conditions:

$$\int_{\mathbb{R}^N} \rho_g(q, p) dp = \int_{\mathbb{R}^N} \chi_q^{(g)}(q') \langle q' | \rho | q' \rangle dq' \quad (1.7a)$$

$$\int_{\mathbb{R}^N} \rho_g(q, p) dq = \int_{\mathbb{R}^N} \chi_p^{(g)'}(p') \langle p' | \rho | p' \rangle dp' \quad (1.7b)$$

which are in keeping with (1.1) and the fact that $\langle q' | \rho | q' \rangle$ and $\langle p' | \rho | p' \rangle$ are probability densities at sharp position and momentum values, respectively.

A particularly important case of representations (1.2) for ρ occurs when

$$g^{(s)} = |e^{(s)}\rangle \langle e^{(s)}|, \quad s = (s_1, s_2, \dots, s_N), \quad s_1, s_2, \dots, s_N > 0 \quad (1.8)$$

$$e^{(s)}(x) = \prod_{\nu=1}^N (\pi \hbar s_\nu^2)^{-1/4} \exp\left(-\frac{x_\nu^2}{2\hbar s_\nu^2}\right), \quad x \in \mathbb{R}^N \quad (1.9)$$

The resulting probability densities $\rho_g(s)(q, p)$ are usually called Husimi transforms (Husimi, 1940), whereas, in the context of the present interpretation, they are referred to as Γ_g -distribution functions (Prugovečki, 1976b). Husimi transforms have already proved useful in extending results in statistical mechanics from the classical realm to the quantum case (McKenna and Frisch, 1965, 1966; Prugovečki, 1978c). Typically, this type of problem requires not only

that quantum states be represented by the probability densities $\rho_g(q, p)$, but also that expectation values of observables, the actions of the generators of motion, etc., be represented in terms of objects directly related to the space $\mathcal{P}(\Gamma_g)$ of probability densities on the stochastic phase space Γ_g .

In Section 2 we present a general method for assigning to an operator A in the Hilbert space \mathcal{H} (and, in particular, to an observable) a function or, in general, a tempered distribution $A_g(q, p)$ so that the following equation holds:

$$\text{Tr}(A\rho) = \int_{\Gamma} A_g(q, p)\rho_g(q, p) dq dp \quad (1.10)$$

Then, in Section 3, we extend this result by showing that a (formal) differential operator $A_I^{(g)}$ can be also assigned to A in such a manner that

$$A_I^{(g)}\rho_g(q, p) = (A\rho)_g(q, p) \quad (1.11)$$

The methods presented are applicable in general, but we illustrate them primarily on the case where g is of the form (1.8). In that instance, as an important special application, we use the derived results to obtain a Bloch equation, from which the Husimi transform of the canonical equilibrium state is then computed by expressing it as a power series in \hbar .

2. The $\mathcal{P}(\Gamma_g)$ Representation Space

Let us denote by Γ_g the set of all stochastic phase space points (\hat{q}, \hat{p}) , $q, p \in \mathbb{R}^N$, with \hat{q} and \hat{p} given by (1.5) and (1.6). We shall refer to Γ_g as the *stochastic phase space* corresponding to g and shall designate by $\mathcal{P}(\Gamma_g)$ the set of all Γ_g -distribution functions (1.2) obtained as ρ varies over all density operators in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^N)$. The family $\mathcal{P}(\Gamma_g)$ of probability densities forms a continuous phase-space representation of quantum mechanics on $L^2(\mathbb{R}^N)$ (in the sense of Ali and Prugovečki, 1977a) if and only if the mapping $\rho \mapsto \rho_g(q, p)$ satisfies the criterion of informational completeness, i.e., if and only if it is one-to-one.

It has been established by Ali and Prugovečki (1977b, Appendix A), that informational completeness is present if and only if $\tilde{g}_w(q, p) \neq 0$ almost everywhere in Γ , where, in general, for any trace-class operator X , we write

$$\tilde{X}_w(q, p) = \text{Tr}[U^*(q, p)X] \quad (2.1)$$

Let $L^2(\Gamma)$ be the Hilbert space of all complex-valued functions on Γ that are square integrable with respect to the measure

$$d\Gamma = h^{-N} dq dp \quad (2.2)$$

If we denote by $\tilde{f}(q, p)$ the symplectic Fourier transform of $f(q, p) \in L^2(\Gamma)$:

$$\tilde{f}(q, p) = \text{l.i.m.} \int_{\Gamma} \exp [i/\hbar(q \cdot p' - p \cdot q')] f(q', p') d\Gamma' \quad (2.3)$$

then equation (A.12) in the aforementioned Appendix A is observed to be equivalent to the statement that

$$h^N \tilde{X}_g(q, p) = \tilde{g}_w(q, p) \tilde{X}_w(q, p) \tag{2.4}$$

where, as a generalization of (1.2), we set

$$X_g(q, p) = h^{-N} \text{Tr} [U(q, p)gU^*(q, p)X] \tag{2.5}$$

and the bar denotes complex conjugation. Setting $g = X$ in (2.4) we obtain

$$\tilde{g}(q, p) \equiv \tilde{g}_g(q, p) = h^{-N} |\tilde{g}_w(q, p)|^2 \tag{2.6}$$

so that, by informational completeness

$$\tilde{g}(q, p) > 0 \tag{2.7}$$

almost everywhere in Γ .

Noting that the inverse symplectic Fourier transform of $\tilde{f}(q, p)$ satisfies

$$f(q, p) = \int_{\Gamma} \exp [i/\hbar(q \cdot p' - p \cdot q')] \tilde{f}(q', p') d\Gamma' \tag{2.8}$$

we easily establish that $\tilde{X}_w(q, p)$ in (2.1) coincides with the symplectic Fourier transform of the Weyl transform $X_w(q, p)$ as defined by Pool (1966). Since the symplectic Fourier transform preserves the norm in $L^2(\Gamma)$:

$$\|f\|_{\Gamma} = \|\tilde{f}\|_{\Gamma}, \quad \|f\|_{\Gamma}^2 = \int_{\Gamma} |f(q, p)|^2 d\Gamma \tag{2.9}$$

and therefore it is one-to-one, we conclude that the following holds true.

Theorem 2.1. If the mapping $\rho \mapsto \rho_g(q, p)$ is informationally complete, there is a one-to-one mapping $\rho_g(q, p) \mapsto \rho_w(q, p)$ of $\mathcal{P}(\Gamma_g)$ onto the space $\mathcal{P}_w(\Gamma)$ of all Weyl transforms of density operators, so that the corresponding symplectic Fourier transforms $\tilde{\rho}_g(q, p)$ and $\tilde{\rho}_w(q, p)$ satisfy (2.4).

Since any Hilbert-Schmidt operator X can be recovered from $\tilde{X}_w(q, p)$ (Pool, 1966) by setting

$$X = \int_{\Gamma} U(q, p) \tilde{X}_w(q, p) d\Gamma \tag{2.10}$$

where the convergence of the above Bochner integral is in the weak operator sense, we observe that for any given stochastic phase-space representation $\mathcal{P}(\Gamma_g)$, the density operator ρ can be recovered from the corresponding Γ_g -distribution function $\rho_g(q, p)$:

$$\rho = \int_{\Gamma} U(q, p) \tilde{\rho}_g(q, p) [\tilde{g}_w(q, p)]^{-1} dq dp \tag{2.11}$$

Using the convenient notation

$$\hat{f}(q, p) = \bar{f}(-q, -p) \tag{2.12}$$

and taking the symplectic Fourier transform of both sides of (2.6), we obtain

$$g(q, p) = h^{-N}(g_w * \hat{g}_w)(q, p) = g(-q, -p) \tag{2.13}$$

where the asterisk denotes the convolution:

$$(f * g)(q, p) = \int f(q', p')g(q - q', p - p') d\Gamma' \tag{2.14}$$

Since we easily obtain from (2.1) that $|\tilde{X}_w(q, p)|$ is an even function of q and p , we arrive at the conclusion that both $g(q, p)$ and $\tilde{g}(q, p)$ are even, positive semidefinite, and continuous functions.

Another feature of the generator g that we shall need in the sequel is the differentiability of $\tilde{g}(q, p)$. Writing in accordance with (1.3) and (2.1)

$$\tilde{g}_w(q, p) = \text{Tr} \left[\exp \left(-\frac{i}{\hbar} p \cdot Q \right) g \exp \left(\frac{i}{\hbar} q \cdot P \right) \right] \tag{2.15}$$

and assuming that in the spectral decomposition

$$g = \sum_{j=1}^{\infty} |e_j\rangle \lambda_j \langle e_j|, \quad \sum_j \lambda_j = 1, \quad \lambda_j \geq 0 \tag{2.16}$$

all the elements of the orthonormal basis e_1, e_2, \dots , are in the domains of definition of

$$P^k = P_1^{k_1} \dots P_N^{k_N}, \quad Q^l = Q_1^{l_1} \dots Q_N^{l_N} \tag{2.17}$$

we conclude that

$$\frac{\partial^{l_1 + \dots + l_N}}{\partial q^{k_1} \partial p^{l_1}} \tilde{g}_w(q, p) = (-1)^{|l|} \left(\frac{i}{\hbar} \right)^{l_1 + \dots + l_N} \text{Tr} \left[\exp \left(-\frac{i}{\hbar} p \cdot Q \right) Q^l g P^k \exp \left(\frac{i}{\hbar} q \cdot P \right) \right] \tag{2.18}$$

and therefore, that the partial derivatives of $\tilde{g}(q, p)$ also exist.

Now we turn our attention to proving that a representation $A_g(q, p)$ satisfying (1.10) exists for any observable A . For that purpose we introduce the space

$$\tilde{\mathcal{S}}_g(\mathbb{R}^{2N}) = \{ \tilde{g}_w(q, p) \tilde{f}(q, p) \mid \tilde{f} \in \mathcal{S}(\mathbb{R}^{2N}) \} \tag{2.19}$$

of test functions obtained by letting \tilde{f} vary over the Schwartz space $\mathcal{S}(\mathbb{R}^{2N})$. We equip $\tilde{\mathcal{S}}_g(\mathbb{R}^{2N})$ with the natural topology induced by the mapping $\tilde{f} \mapsto \tilde{g}_w \cdot \tilde{f}$ (i.e., the topology under which this mapping is a homeomorphism). Similarly, we denote by $\mathcal{S}_g(\mathbb{R}^{2N})$ the space of test functions f which are the symplectic Fourier transforms (2.8) of $\tilde{f} \in \tilde{\mathcal{S}}_g$, and we equip \mathcal{S}_g with the natural topology induced by this transform.

Theorem 2.2. To every operator A on $L^2(\mathbb{R}^N)$, which is either bounded or unbounded and symmetric with domain containing $\mathcal{S}(\mathbb{R}^N)$, corresponds a unique distribution $A_g(q, p)$ on $\mathcal{S}'_g(\mathbb{R}^{2N})$ for which

$$\langle \phi | A \psi \rangle = \int A_g(q, p) X_g^{\phi, \psi}(q, p) dq dp \tag{2.20}$$

whenever the function

$$X_g^{\phi, \psi}(q, p) = h^{-N} \langle \phi | U(q, p) g U^*(q, p) \psi \rangle \tag{2.21}$$

belongs to $\mathcal{S}'_g(\mathbb{R}^{2N})$, and in particular if $\phi, \psi \in \mathcal{S}(\mathbb{R}^N)$. Furthermore,

$$\tilde{A}_g(q, p) = [\tilde{g}_w(q, p)]^{-1} \tilde{A}_w(q, p) \tag{2.22}$$

where, in general, $\tilde{A}_w(q, p)$ is a tempered distribution on $\mathcal{S}(\mathbb{R}^{2N})$, and in particular, if A is Hilbert-Schmidt $\tilde{A}_w \in L^2(\mathbb{R}^{2N})$ and $\tilde{A}_g(q, p)$ is an almost-everywhere-defined function. If A is symmetric, the distribution $A_g(q, p)$ is real.

Proof. To prove the first part of the theorem, we note that in view of the linear isometry (Pool, 1966) between the Hilbert spaces of the set of all Hilbert-Schmidt operators X , and the set of their Weyl transforms $X_w(q, p)$, if A is a Hilbert-Schmidt operator, then for any $\phi, \psi \in \mathcal{H} [= L^2(\mathbb{R}^N)]$,

$$\begin{aligned} \langle \phi | A \psi \rangle &= \text{tr} [A | \psi \rangle \langle \phi |] \\ &= \int_{\Gamma} \tilde{A}_w(-q, -p) \tilde{X}_w^{\phi, \psi}(q, p) \exp\left(\frac{i}{\hbar} q \cdot p\right) d\Gamma \end{aligned} \tag{2.23}$$

where, in accordance with equation (2.1),

$$\tilde{X}_w^{\phi, \psi}(q, p) = \langle \phi | U^*(q, p) \psi \rangle \tag{2.24}$$

In obtaining (2.23) we have used the definitions of the scalar product on $L^2(\Gamma)$ and that of two Hilbert-Schmidt operators, and the fact that if X^* is adjoint to X , then

$$\tilde{X}_w^*(q, p) = \tilde{X}_w(-q, -p) \cdot \exp\left(-\frac{i}{\hbar} q \cdot p\right) \tag{2.25}$$

By Cressman (1976), (2.23) may be extended to the case where A is any operator, bounded or unbounded and symmetric, with domain containing $\mathcal{S}(\mathbb{R}^N)$. In that case $\tilde{A}_w(q, p)$ is in general a tempered distribution, and ϕ, ψ have to be chosen so that $\tilde{X}_w^{\phi, \psi} \in \mathcal{S}'(\mathbb{R}^N)$ —i.e., so that $\phi, \psi \in \mathcal{S}(\mathbb{R}^N)$. Upon using (2.24) in (2.23) we get

$$\langle \phi | A \psi \rangle = \int \tilde{A}_w(-q, -p) [\tilde{g}_w(q, p)]^{-1} \tilde{X}_g^{\phi, \psi}(q, p) \cdot \exp\left(\frac{i}{\hbar} q \cdot p\right) dq dp \tag{2.26}$$

where now $\tilde{X}_g^{\phi, \psi} \in \tilde{\mathcal{S}}_g(\mathbb{R}^{2N})$. Using (2.25) and the fact that $g = g^*$, we may rewrite (2.26) as

$$\langle \phi | A \psi \rangle = \int \tilde{A}_g(-q, -p) \tilde{X}_g^{\phi, \psi}(q, p) dq dp \tag{2.27}$$

where we have set

$$\tilde{A}_g(q, p) = [\tilde{g}_w(q, p)]^{-1} \tilde{A}_w(q, p) \tag{2.28}$$

Since \tilde{A}_w is unique, it follows that \tilde{A}_g is indeed a unique distribution on $\tilde{\mathcal{S}}_g(\mathbb{R}^{2N})$. Finally, upon using the definition of the symplectic Fourier transform of a distribution,

$$\int \tilde{A}_g(-q, -p) \tilde{f}(q, p) dq dp = \int A_g(q, p) f(q, p) dq dp \tag{2.29}$$

[which is easily checked to be in agreement with Parseval's inequality when $A_g \in L^2(\mathbb{R}^{2N})$], we obtain (2.20), with A_g in general a unique distribution on $\tilde{\mathcal{S}}_g(\mathbb{R}^{2N})$.

To prove the reality of $A_g(q, p)$ when $A = A^*$, we note first that if $f \in \tilde{\mathcal{S}}(\mathbb{R}^{2N})$, then using an extended version of (2.10) and the uniqueness of the distribution \tilde{X}_w , we have

$$\int \tilde{X}_w^*(q, p) f(q, p) dq dp = \int \tilde{X}_w(-q, -p) \exp\left(-\frac{i}{\hbar} q \cdot p\right) \cdot f(q, p) dq dp \tag{2.30}$$

in analogy with (2.25). Hence setting $X = A = A^*$, and taking f in $\tilde{\mathcal{S}}_g(\mathbb{R}^{2N})$ we get, using equation (2.28),

$$\int \tilde{A}_g(q, p) f(q, p) dq dp = \int \tilde{A}_w(-q, -p) [\tilde{g}_w(q, p)]^{-1} \exp\left(-\frac{i}{\hbar} q \cdot p\right) \times f(q, p) dq dp \tag{2.31}$$

On using (2.25) in (2.31) we get

$$\int \tilde{A}_g(q, p) f(q, p) dq dp = \int \tilde{A}_g(-q, -p) f(q, p) dq dp \tag{2.32}$$

Equation (2.25) is easily seen to imply that for $f \in \tilde{\mathcal{S}}_g(\mathbb{R}^{2N})$ and f positive,

$$\int A_g(q, p) f(q, p) dq dp = \overline{\int A_g(q, p) f(q, p) dq dp} \tag{2.33}$$

□

As an example of a Γ_g -distribution function, let us consider the $\mathcal{P}(\Gamma_g)$ representative of the canonical state

$$\rho^{(\beta)} = Z_\beta^{-1} e^{-\beta H}, \quad \beta = \frac{1}{kT} \tag{2.34}$$

$$Z_\beta = \text{Tr } e^{-\beta H} \tag{2.35}$$

where g is given by equations (1.8) and (1.9) and H is the N -dimensional anisotropic oscillator Hamiltonian

$$H = \frac{1}{2} \sum_{\nu=1}^N (P_{\nu}^2 + \omega_{\nu}^2 Q_{\nu}^2) \tag{2.36}$$

In that case the Weyl transform of $\rho^{(\beta)}$ can be computed explicitly (Emch, 1976):

$$\rho_w^{(\beta)}(q, p) = \prod_{\nu=1}^N \exp \left[-\frac{1}{4} \theta_{\nu} \left(\frac{\omega_{\nu}}{\hbar^2} q_{\nu}^2 + \frac{1}{\omega_{\nu} \hbar^2} p_{\nu}^2 \right) - \frac{i}{2\hbar} q_{\nu} p_{\nu} \right] \tag{2.37}$$

$$\theta_{\nu} = \coth \left(\frac{\beta \omega_{\nu}}{2} \right) \tag{2.38}$$

Since it is easily established that

$$\tilde{g}_w^{(s)}(q, p) = \prod_{\nu=1}^N \exp \left[-\frac{1}{4\hbar} \left(\frac{q_{\nu}^2}{s_{\nu}^2} + s_{\nu}^2 p_{\nu}^2 \right) - \frac{i}{2\hbar} q_{\nu} p_{\nu} \right] \tag{2.39}$$

we obtain by (2.4) and (2.8)

$$\rho_{g^{(s)}}^{(\beta)}(q, p) = \pi^{-N} \prod_{\nu=1}^N \frac{1}{\sigma_{1\nu} \sigma_{2\nu}} \exp \left(-\frac{q_{\nu}^2}{\sigma_{1\nu}^2} - \frac{p_{\nu}^2}{\sigma_{2\nu}^2} \right) \tag{2.40}$$

$$\sigma_{1\nu} = \hbar s_{\nu}^2 + \frac{\theta_{\nu}}{\omega_{\nu}}, \quad \sigma_{2\nu}^2 = \frac{\hbar}{s_{\nu}^2} + \theta_{\nu} \omega_{\nu} \tag{2.41}$$

It is also interesting to note that

$$\tilde{g}^{(s)}(q, p) = h^{-N} \prod_{\nu=1}^N \exp \left[-\frac{1}{2\hbar} \left(\frac{q_{\nu}^2}{s_{\nu}^2} + s_{\nu}^2 p_{\nu}^2 \right) \right] = g^{(s)}(q, p) \tag{2.42}$$

3. The $\mathcal{P}(\Gamma_g)$ Representation of Superoperators

The distribution $A_g(q, p)$ enables us to compute directly within the $\mathcal{P}(\Gamma_g)$ formalism the expectation value $\langle A \rangle_{\rho}$ in (1.10) for the observable A . However, occasionally the action of the superoperators A_l , A_r and \mathbf{A} on ρ

$$A_l \rho = A \rho, \quad A_r \rho = \rho A, \quad \mathbf{A} \rho = \frac{1}{2} [A, \rho] \tag{3.1}$$

can be of independent interest, as we shall see later on when we discuss the Bloch equation. Furthermore, to deal with the Liouville equation

$$i \partial / \partial t \rho(t) = H \rho(t), \quad H \rho = \hbar^{-1} [H, \rho] \tag{3.2}$$

directly within the $\mathcal{P}(\Gamma_g)$ formalism we have to be able to express the action of the superoperator $-iH$ on ρ in terms of a Liouville operator $L^{(g)}$ acting on $\rho_g(q, p)$ in such a manner that

$$L^{(g)}\rho_g(q, p) = -i\text{Tr}[U(q, p)gU^*(q, p)(H\rho)] \tag{3.3}$$

The manner to proceed is by noting that in accordance with (2.4) and (2.8)

$$(A\rho)_g(q, p) = \int_{\Gamma} \exp\left[-\frac{i}{\hbar}(q' \cdot p - p' \cdot q)\right] \tilde{g}_w(q', p')(A\rho)_w(q', p') dq' dp' \tag{3.4}$$

Upon using the easily verified relation

$$(A\rho)_w(q, p) = \int_{\Gamma} \exp\left[-\frac{i}{\hbar}q'(p - p')\right] \tilde{A}_w(q', p') \tilde{\rho}_w(q - q', p - p') d\Gamma' \tag{3.5}$$

which is to be interpreted in an appropriate distribution theoretic sense, (3.4) yields

$$\begin{aligned} A_f^{(g)}\rho_g(q, p) &= (A\rho)_g(q, p) = h^{-N} \int \exp\left[\frac{i}{\hbar}(q \cdot p_1 - p \cdot q_1) - \frac{i}{\hbar}q_2(p_1 - p_2)\right] \\ &\times \tilde{g}_w(q_1, p_1) \tilde{g}_w(q_2, p_2) [\tilde{g}_w(q_1 - q_2, p_1 - p_2)]^{-1} \\ &\times \tilde{A}_g(q, p) \tilde{\rho}_g(q_1 - q_2, p_1 - p_2) dq_1 dq_2 dp_1 dp_2 \end{aligned} \tag{3.6}$$

To exhibit $A_f^{(g)}$ as a formal differential operator (of finite or infinite order) we shall assume throughout this section that both $\tilde{g}_w(q, p)$ and $[\tilde{g}(q, p)]^{-1}$ are boundary values of entire analytic functions in $2N$ complex variables. For example this is the case with $g^{(s)}$ as in equation (1.8), for which $\tilde{g}_w(s)(q, p)$ is given by (2.39). As a matter of fact, since by (2.18) the coefficients a_{kl} of the Taylor expansion of $\tilde{g}_w(q, p)$ at $q = p = 0$ are

$$a_{kl} = \frac{(-1)^l}{k!l!} \left(\frac{i}{\hbar}\right)^{|k+l|} \text{Tr}(Q^l g P^k) \tag{3.7}$$

we see that there is a large class of representation generators g satisfying this requirement.

With this restriction in mind, we notice that the right-hand side of (3.6) involves symplectic Fourier transforms of expressions of the type

$$h = fh_1 \tag{3.8}$$

where h and h_1 are in general distributions on $\tilde{\mathcal{F}}_g$ and f is the boundary value of an entire analytic function. In case h_1 is itself a function on Γ , the product distribution h becomes simply another function h on Γ , and we may write

$$h(q, p) = f(q, p)h_1(q, p) \tag{3.9}$$

Furthermore, f has the Taylor expansion

$$f(q, p) = \sum_{k,l} c_{kl} q^k p^l \tag{3.10}$$

$$q^k = q_1^{k_1} q_2^{k_2} \dots q_N^{k_N}, \quad p^l = p_1^{l_1} p_2^{l_2} \dots p_n^{l_n} \tag{3.11}$$

Let us formally write

$$f\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) = \sum_{k,l} c_{kl} \frac{\partial^{|k+l|}}{\partial q^k \partial p^l} \tag{3.12}$$

in the obvious standard notation. We shall then write the symplectic Fourier transform \tilde{h} of the distribution h in the form

$$\tilde{h} = f\left(i\hbar \frac{\partial}{\partial p}, -i\hbar \frac{\partial}{\partial q}\right) \tilde{h}_1 \tag{3.13}$$

Actually, taking a bit of liberty with the notation, we shall write

$$\tilde{h}(q, p) = f\left(i\hbar \frac{\partial}{\partial p}, -i\hbar \frac{\partial}{\partial q}\right) \tilde{h}_1(q, p) \tag{3.14}$$

For many functions h_1 (e.g., when \tilde{h}_1 is a polynomial in q, p) $f(i\hbar(\partial/\partial p), -i\hbar(\partial/\partial q))$ can be considered to be a standard differential operator. Otherwise we shall interpret the right-hand side of (3.14) as being simply the symplectic Fourier transform of the distribution h .

Using the notation introduced in (3.14), equation (3.6) may be put in the compact form

$$\begin{aligned} A_l^{(g)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) \rho_g(q, p) &\equiv (A\rho)_g(q, p) \\ &= h^N \exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{12}\right] \tilde{g}_w\left(-i\hbar \frac{\partial}{\partial p}, i\hbar \frac{\partial}{\partial q}\right) \\ &\quad \times \left[\tilde{g}_w\left(i\hbar \frac{\partial}{\partial p}, -i\hbar \frac{\partial}{\partial q}\right) A_g(q, p)\right] \\ &\quad \times \left[\tilde{g}_w^{-1}\left(i\hbar \frac{\partial}{\partial p} - i\hbar \frac{\partial}{\partial q}\right) \rho_g(q, p)\right] \end{aligned} \tag{3.15}$$

where for two functions f, g on Γ

$$\begin{aligned} &\exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{12}\right] f(q, p) g(q, p) \\ &= \exp\left(-i\hbar \frac{\partial}{\partial p_1} \cdot \frac{\partial}{\partial q_2}\right) f(q_1, p_1) g(q_2, p_2) \Bigg|_{\substack{q_1 = q_2 = q \\ p_1 = p_2 = p}} \end{aligned} \tag{3.16}$$

An expression similar to (3.15) has also been obtained by Agarwal and Wolf (1970). The operator $A_l^{(g)}$, which formally resembles a differential operator may now be written as

$$A_l^{(g)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) = \exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{12}\right] \bar{g}_w\left(-i\hbar\frac{\partial}{\partial p}, i\hbar\frac{\partial}{\partial q}\right) \\ \times \left[\tilde{g}_w\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) A_g(q, p)\right] \bar{g}^{-1}\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) \quad (3.17a)$$

and similarly,

$$A_r^{(g)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) = \exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{21}\right] \bar{g}_w\left(-i\hbar\frac{\partial}{\partial p}, i\hbar\frac{\partial}{\partial q}\right) \\ \times \left[\tilde{g}_w\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) A_g(q, p)\right] \bar{g}^{-1}\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) \quad (3.17b)$$

Thus the operator $L^{(g)}$ introduced in (3.3) becomes

$$L^{(g)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) = -\frac{i}{\hbar}\left\{\exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{12}\right] - \exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{21}\right]\right\} \\ \times \bar{g}_w\left(-i\hbar\frac{\partial}{\partial p}, i\hbar\frac{\partial}{\partial q}\right) \left[\tilde{g}_w\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) H_g(q, p)\right] \\ \times \bar{g}_w^{-1}\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) \quad (3.18)$$

and finally,

$$A^{(g)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) = \frac{1}{2}\left\{\exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{12}\right] + \exp\left[-i\hbar\left(\frac{\partial}{\partial p}, \frac{\partial}{\partial q}\right)_{21}\right]\right\} \\ \times \bar{g}_w\left(-i\hbar\frac{\partial}{\partial p}, i\hbar\frac{\partial}{\partial q}\right) \left[\tilde{g}_w\left(i\hbar\frac{\partial}{\partial p}, -i\hbar\frac{\partial}{\partial q}\right) A_g(q, p)\right] \\ \times \bar{g}_w^{-1}\left(i\hbar\frac{\partial}{\partial q}, -i\hbar\frac{\partial}{\partial q}\right) \quad (3.19)$$

where we have defined the operator $A^{(g)}$ as

$$A^{(g)}\rho_g(q, p) = \text{Tr}[U(q, p)gU^*(q, p)A\rho] \quad (3.20)$$

with A as in (3.1).

Equations (3.18) and (3.19) look somewhat complicated. However, in specific instances the expressions collapse into fairly simple forms. In this connection, it is instructive to study examples where the operators $A^{(g)}$ are polynomials in $\partial/\partial q$ and $\partial/\partial p$. For this purpose it is useful to rewrite (3.19) in the form

$$\begin{aligned}
 A^{(g)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) \rho_g(q, p) &= \frac{1}{2} \left[\exp\left(-i\hbar \frac{\partial}{\partial p_1} \cdot \frac{\partial}{\partial q_2}\right) + \exp\left(-i\hbar \frac{\partial}{\partial p_2} \cdot \frac{\partial}{\partial q_1}\right) \right] \\
 &\quad \times \tilde{g}_w \left(-i\hbar \frac{\partial}{\partial p_1} - i\hbar \frac{\partial}{\partial p_2}, i\hbar \frac{\partial}{\partial q_1} + i\hbar \frac{\partial}{\partial q_2} \right) \tilde{g}_w \left(i\hbar \frac{\partial}{\partial p_1}, -i\hbar \frac{\partial}{\partial q_1} \right) \\
 &\quad \times \tilde{g}_w^{-1} \left(i\hbar \frac{\partial}{\partial p_2}, -i\hbar \frac{\partial}{\partial q_2} \right) A_g(q_1, p_1) \rho_g(q_2, p_2) \Big|_{\substack{q_1 = q_2 = q \\ p_1 = p_2 = p}}
 \end{aligned} \tag{3.21}$$

where use has been made of the fact that if f and g are two functions on Γ , then

$$\frac{\partial^n}{\partial q^n} [f(q, p)g(q, p)] = \left(\frac{\partial}{\partial q_1} + \frac{\partial}{\partial q_2} \right)^n f(q_1, p_1)g(q_2, p_2) \Big|_{\substack{q_1 = q_2 = q \\ p_1 = p_2 = p}} \tag{3.22}$$

and similarly for $\partial^n/\partial p^n$.

Consider now the case where \tilde{g}_w is the one given by (2.39), and $A_g(q, p)$ is a polynomial in q and p . Then it is easy to verify that (writing $A^{(s)}$ for $A^{(g^{(s)})}$, A_s for $A_{g^{(s)}}$, etc.)

$$\begin{aligned}
 A^{(s)}\left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p}\right) \rho_s(q, p) &= \frac{1}{2} \left\{ \exp\left[\frac{i\hbar}{2} \left(\frac{\partial}{\partial q_1} \cdot \frac{\partial}{\partial p_2} - \frac{\partial}{\partial p_1} \cdot \frac{\partial}{\partial q_2} \right) \right. \right. \\
 &\quad \left. \left. + \exp\left[-\frac{i\hbar}{2} \left(\frac{\partial}{\partial q_1} \cdot \frac{\partial}{\partial p_2} - \frac{\partial}{\partial p_1} \cdot \frac{\partial}{\partial q_2} \right) \right] \right\} \\
 &\quad \times \exp\left[\frac{\hbar}{2} \left(\frac{1}{s^2} \frac{\partial^2}{\partial p_1^2} + s^2 \frac{\partial^2}{\partial q_1^2} + \frac{1}{s^2} \frac{\partial}{\partial p_1} \cdot \frac{\partial}{\partial p_2} + s^2 \frac{\partial}{\partial q_1} \cdot \frac{\partial}{\partial q_2} \right) \right] \\
 &\quad \times A_s(q_1, p_1) \rho_s(q_2, p_2) \Big|_{\substack{q_1 = q_2 = q \\ p_1 = p_2 = p}}
 \end{aligned} \tag{3.23}$$

where

$$\frac{1}{s^2} \frac{\partial^2}{\partial p^2} = \sum_{\nu=1}^N \frac{1}{s_\nu^2} \frac{\partial^2}{\partial p_\nu^2} \tag{3.24a}$$

$$s^2 \frac{\partial}{\partial q_1} \cdot \frac{\partial}{\partial q_2} = \sum_{\nu=1}^N s_\nu^2 \frac{\partial^2}{\partial q_{\nu 1} \partial q_{\nu 2}} \quad (3.24b)$$

etc. Thus, since $A_s(q, p)$ is assumed to be a polynomial, we get

$$\begin{aligned} \mathbf{A}^{(s)} \left(\frac{\partial}{\partial q}, \frac{\partial}{\partial p} \right) A_s(q, p) &= \frac{1}{2} \exp \left[\frac{\hbar}{2} \left(\frac{1}{s^2} \frac{\partial^2}{\partial p_1^2} + s^2 \frac{\partial^2}{\partial q_1^2} \right) \right] \\ &\times \left[A_s \left(q_1 + \frac{i\hbar}{2} \frac{\partial}{\partial p_2} + \frac{\hbar s^2}{2} \frac{\partial}{\partial q_2}, p_1 - \frac{i\hbar}{2} \frac{\partial}{\partial q_2} + \frac{\hbar}{2s^2} \frac{\partial}{\partial p_2} \right) \right. \\ &+ A_s \left(q_1 - \frac{i\hbar}{2} \frac{\partial}{\partial p_2} + \frac{\hbar s^2}{2} \frac{\partial}{\partial q_2}, p_1 + \frac{i\hbar}{2} \frac{\partial}{\partial q_2} + \frac{\hbar}{2s^2} \frac{\partial}{\partial p_2} \right) \left. \right] \\ &\times \rho_s(q_2, p_2) \Big|_{\substack{q_1 = q_2 = q \\ p_1 = p_2 = p}} \quad (3.25) \end{aligned}$$

where by an expression of the type $(\hbar s^2/2)(\partial/\partial q)$, inside the second square bracket we mean a vector differential operator with components $(\hbar s_\nu^2/2)(\partial/\partial q_\nu)$, and so on.

Consider the case where $A = Q_\nu$, the position operator. Then, using the formal relation

$$\text{Tr}[U^*(q', p')U(q, p)] d\Gamma = \delta(q - q', p - p') dq dp \quad (3.26)$$

it is easy to verify that

$$\tilde{A}_w(q, p) d\Gamma = i\hbar \frac{\partial}{\partial p_\nu} \delta(q, p) dq dp \quad (3.27)$$

so that

$$A_s(q, p) = q_\nu \quad (3.28)$$

and hence, on using (3.25),

$$\mathbf{Q}_\nu^{(s)} = q_\nu + \frac{\hbar s_\nu^2}{2} \frac{\partial}{\partial q_\nu} \quad (3.29a)$$

Similarly, for the momentum operator P_ν we get

$$\mathbf{P}_\nu^{(s)} = p_\nu + \frac{\hbar s_\nu^2}{2} \frac{\partial}{\partial p_\nu} \quad (3.29b)$$

From the form of (3.25) it is clear that $\mathbf{A}^{(s)}(\partial/\partial q, \partial/\partial p)$ is a polynomial in $q, p, \partial/\partial q$, and $\partial/\partial p$, as is seen for example from equations (3.29), or, for example, from the corresponding expression obtained for the free Hamiltonian

$$H_0 = \sum_{\nu=1}^N \frac{P_\nu}{2m_\nu} \tag{3.30}$$

in which case (cf. Prugovečki, 1978b)

$$\mathbf{H}_0^{(s)} = \sum_{\nu=1}^N \left[\frac{p_\nu^2}{2m_\nu} + \frac{\hbar}{2s_\nu^2 m_\nu} \left(\frac{1}{2} + p_\nu \frac{\partial}{\partial p_\nu} \right) + \frac{\hbar^2}{8m_\nu} \left(\frac{1}{s_\nu^4} \frac{\partial}{\partial p_\nu^2} - \frac{\partial^2}{\partial q_\nu^2} \right) \right] \tag{3.31}$$

We observe that the leading term on the right-hand side of equation (3.31), containing no powers in \hbar , coincides with the classical kinetic energy

$$E_0(p) = \sum_{\nu=1}^N \frac{p_\nu^2}{2m_\nu} \tag{3.32}$$

and indeed this same feature is also shared by the expressions for $\mathbf{Q}_\nu^{(s)}$ and $\mathbf{P}_\nu^{(s)}$ in (3.29). On the other hand, if A is an operator for which $A_s(q, p)$ is not a polynomial, such as for example an interaction given by a general potential $V(x)$, it will no longer be the case that $\mathbf{A}^{(s)}$ is a polynomial in $q, p, \partial/\partial q$, and $\partial/\partial p$. If $V(x)$ is an entire function, then the corresponding interaction Hamiltonian operator $\mathbf{H}_I^{(s)}$ on $\mathcal{P}(\Gamma_s)$, and the Liouville operator $L_I^{(s)} = -i \mathbf{H}_I^{(s)}$, are going to be differential operators of, in general, infinite order (Prugovečki, 1978a, b). If, however, $V(x)$ is not an entire function, then $\mathbf{H}_I^{(s)}$ and $L_I^{(s)}$ can only be represented as integral operators (Ali and Prugovečki, 1977b, Appendix B).

4. The Bloch Equation for the $\mathcal{P}(\Gamma_s)$ Representation of Canonical States

In Section 2 we could perform the explicit computation of the Γ_s -distribution function (i.e., Husimi transform) of the canonical state $\rho^{(\beta)}$ due to the simple form of the chosen Hamiltonian (2.36). In general, however, one has to rely on perturbational methods in order to compute $\rho_g^{(\beta)}(q, p)$. The method we adopt in this section is in essence the same as the one used in similar computations of the Wigner transform, i.e., it coincides with the approach initiated by Wigner (1932) and Kirkwood (1933), and perfected by some other authors (Saenz and O'Rourke, 1955; Oppenheim and Ross, 1957). It consists of computing in the expansion

$$I^{(\beta)} \equiv \exp(-\beta H) = \exp(-\beta E) [1 + \hbar \chi_1(\beta) + \hbar^2 \chi_2(\beta) + \dots] \tag{4.1}$$

$$E(q, p) = \frac{p_\nu^2}{2m_\nu} + V(q) \tag{4.2}$$

the terms $\chi_1(\beta), \chi_2(\beta), \dots$ by iteration, thus obtaining for $I^{(\beta)}$, as well as for the partition function Z_β , approximations to different orders of \hbar . The method is considered reliable at high temperatures. Alternative methods, such as expansions in powers of the interaction term (Chester, 1954), can be adapted with equal ease to the present case.

For a system of $N/3$ (nonidentical) particles enclosed in a vessel of volume \mathcal{V} , we can use the defining formula (1.2) for $I^{(\beta)}$ to recast its $\mathcal{P}(\Gamma_s)$ representative into the form

$$I_s^{(\beta)}(q, p) = \hbar^{-N} \langle e_{q,p}^{(s)} | I^{(\beta)} e_{q,p}^{(s)} \rangle, \quad e_{q,p}^{(s)} = U(q, p) e^{(s)} \quad (4.3)$$

and then compute $I_s^{(\beta)} = I_s^{(\beta)}(s)$ explicitly. We obtain

$$I_s^{(\beta)}(q, p) = \prod_{\nu=1}^N \left[\hbar^2 \left(1 + \frac{\beta \hbar}{2m_\nu s_\nu^2} \right) \right]^{-1/2} \exp \left(-\beta \frac{p_\nu^2}{2m_\nu + \beta \hbar / s_\nu^2} \right) \quad (4.4)$$

where q is essentially restricted to the interior of the vessel. The corresponding partition function is

$$Z_\beta = \int I_s^{(\beta)}(q, p) dq dp = \mathcal{V}^{-N/3} \prod_{\nu=1}^N \left(\frac{2\pi m_\nu}{\beta \hbar^2} \right)^{1/2} \quad (4.5)$$

and we note that in the limit $s_\nu \rightarrow \infty$, namely, for stochastic points that are sharp in momentum, we recover from

$$\rho_s^{(\beta)}(q, p) = I_s^{(\beta)}(q, p) / Z_\beta(q, p) \quad (4.6)$$

the classical expression for the Γ -distribution function of a canonical system of noninteracting particles, i.e., the Maxwell distribution:

$$\rho_\infty^{(\beta)}(q, p) = \mathcal{V}^{-N/3} \prod_{\nu=1}^N \left(\frac{\beta}{2\pi m_\nu} \right)^{1/2} \exp \left(-\beta \sum_\nu \frac{p_\nu^2}{2m_\nu} \right) \quad (4.7)$$

In the presence of interactions, we use the Bloch equation reexpressed in the $\mathcal{P}(\Gamma_s)$ space,

$$\frac{\partial}{\partial \beta} I_s^{(\beta)}(q, p) = -\mathbf{H}^{(s)} I_s^{(\beta)}(q, p) \quad (4.8)$$

as a means of computing successively the $\mathcal{P}(\Gamma_s)$ representatives $\chi_\alpha(q, p; \beta)$, $\alpha = 1, 2, \dots$, of the different terms in (4.1). Indeed, writing

$$I_s^{(\beta)}(q, p) = \exp[-\beta E(q, p)] \chi(q, p; \beta) \quad (4.9)$$

$$\mathbf{H}^{(s)} = E + \hbar \mathbf{H}_1^{(s)} + \hbar^2 \mathbf{H}_2^{(s)} + \dots \quad (4.10)$$

with $\mathbf{H}^{(s)}$ obtained from (3.21), we obtain from (4.8)

$$\frac{\partial \chi}{\partial \beta} = \exp(\beta E) (\hbar \mathbf{H}_1^{(s)} + \hbar^2 \mathbf{H}_2^{(s)} + \dots) \exp(-\beta E) \chi \quad (4.11)$$

Expressing both sides of (4.11) as power series in \hbar , and equating their coefficients, we arrive at a system of coupled differential equations that can be solved in succession. For example, the first two of these equations are

$$\frac{\partial \chi_1}{\partial \beta} + \exp(\beta E) \mathbf{H}_1^{(s)} \exp(-\beta E) = 0 \tag{4.12}$$

$$\frac{\partial \chi_2}{\partial \beta} + \exp(\beta E) \mathbf{H}_2^{(s)} \exp(\beta E) \chi_2 = -\exp(\beta E) \mathbf{H}_1^{(s)} \exp(-\beta E) \tag{4.13}$$

In order to arrive at a power series expansion (4.10) for $\mathbf{H}^{(s)}$, we make the same technical assumption as in the Wigner transform case (Wigner, 1932), namely, that the potential $V(x)$ is an entire function:

$$V(x) = \sum_{n=0}^{\infty} V_n(q) (x - q)^n, \quad V_n = \frac{1}{n_1! \cdots n_N!} \frac{\partial^{|n|} V}{\partial q_1^{n_1} \cdots \partial q_N^{n_N}} \tag{4.14}$$

The successive computations of $\mathbf{H}_1^{(s)}$, $\mathbf{H}_2^{(s)}$, ... then become a laborious but straightforward task based on the iterative formulas (4.4) of Prugovečki (1978a). For example, in the first order of \hbar we have

$$\mathbf{H}_1^{(s)} = \frac{1}{2} \sum_{\nu} \left[\frac{1}{m_{\nu} s_{\nu}^2} \left(\frac{1}{2} + p_{\nu} \frac{\partial}{\partial p_{\nu}} \right) + s_{\nu}^2 \left(\frac{\partial V}{\partial q_{\nu}} \frac{\partial}{\partial q_{\nu}} + \frac{1}{2} \frac{\partial^2 V}{\partial q_{\nu}^2} \right) \right] \tag{4.15}$$

Consequently, solving (4.12) subject to the boundary condition $\chi_1(q, p) \equiv 0$ in the limit $\beta \rightarrow +0$, we obtain

$$\chi_1(q, p) = \frac{\beta}{4} \sum_{\nu} \left\{ - \left(\frac{1}{m_{\nu} s_{\nu}^2} + s_{\nu}^2 \frac{\partial^2 V}{\partial q_{\nu}^2} \right) + \beta \left[\frac{p_{\nu}^2}{s_{\nu}^2 m_{\nu}^2} + \left(s_{\nu} \frac{\partial V}{\partial q_{\nu}} \right)^2 \right] \right\} \tag{4.16}$$

In the second order, taking $s_1 = \cdots = s_N$ we obtain

$$\begin{aligned} \mathbf{H}_2^{(s)} = & \frac{1}{8} \sum_{\nu} \frac{1}{m_{\nu}} \left(\frac{1}{s_1^4} \frac{\partial^2}{\partial p_{\nu}^2} - \frac{\partial^2}{\partial q_{\nu}^2} \right) + \frac{1}{4} \sum_{\mu, \nu} \frac{\partial^2 V}{\partial q_{\mu} \partial q_{\nu}} \left(s_1^4 \frac{\partial^2}{\partial q_{\mu} \partial p_{\nu}} - \frac{\partial^2}{\partial p_{\mu} \partial p_{\nu}} \right) \\ & + \frac{s_1^4}{8} \sum_{\nu} \left(\frac{\partial^3 V}{\partial q_{\nu}^3} \frac{\partial}{\partial q_{\nu}} + \frac{1}{4} \frac{\partial^4 V}{\partial q_{\nu}^4} \right) + \frac{3s_1^4}{8} \sum_{\nu \neq \mu} \frac{\partial^2 V}{\partial q_{\mu}^2 \partial q_{\nu}} \frac{\partial}{\partial q_{\nu}} \end{aligned} \tag{4.17}$$

and the respective correction χ_2 is of corresponding complexity. However, the computation of the partition function Z_{β} requires that χ be integrated over phase space. As a result, terms that are linear in derivatives of V can be

integrated by parts, and therefore some simplifications can be achieved. For example, to the first order in \hbar

$$Z_\beta \simeq \int \left[1 - \frac{\beta \hbar}{4} \sum_v \left(\frac{1}{m_v s_v^2} - \beta \frac{p_v^2}{s_v^2 m_v^2} \right) \right] \exp [-\beta E(q, p)] dq dp \quad (4.18)$$

It is interesting to note that in contradistinction to the Wigner-transform method, which seems to give a zero contribution in the first order of \hbar (Wigner, 1932; Landau and Lifschitz, 1958) the present Husimi-transform first-order correction does not vanish. That this has to be so is easily confirmed in the limit $V(q) \rightarrow 0$ by taking the explicit expression (4.4) and expanding it in powers of $\beta \hbar$. This discrepancy between the expansions in \hbar based on the Wigner and Husimi transforms, respectively, appears to mark this particular technique since it occurs also in the context of computing quantum corrections to the classical Γ -distribution function of a Brownian particle (cf. McKenna and Frisch, 1966 vs. Resibois and Dagonnier, 1966). Certainly, this matter deserves further consideration.

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