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A Propagator Theory Applied to Wave Mechanics in Phase Space

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The fact that the classical Liouville equation can be analyzed as a dynamical equation in Hilbert-Koopman (HK) space is used in order to develop a perturbative method for the wave mechanics in phase space: an explicit solution of the Liouville equation in qp representation is exhibited. The connection between the solution obtained and the dynamics of correlations is established by computing the qp-kp transformation function in HK space. To elucidate the method, an application is presented and the result compared to that available in the literature.

1. INTRODUCTION

The study of classical statistical mechanics by using methods specially developed in quantum theory has been called by Della Riccia and Wiener (1966) wave mechanics in classical phase space (WMCPS). This formulation of statistical mechanics has a mathematical structure based on the Hilbert-Koopman (HK) space (Koopman, 1931; Misra and Prigogine, 1983; Misra, 1978; George and Prigogine, 1979; Twareque and Prugovečke, 1977; Matos Neto and Vianna 1984, 1985); it has been employed in different versions by Schönberg (1952, 1953*a,b*) in the analysis of Gibbs' paradox, Della Riccia and Wiener (1966) in the study of Brownian motion, and Prigogine and co-workers (Prigogine, 1962, 1980, Prigogine *et al.*, 1973) in several works on nonequilibrium problems.

In the applications of Prigogine formulation the essential step is the expansion of the phase distribution function in a Fourier series in the coordinates $q = (q_1, q_2, q_3, \ldots, q_N)$. In terms of HK space this amounts to a change of representation in which the coordinates q are replaced as

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independent variables by the Fourier indices or "wave vectors" $k = (k_1, k_2, \ldots, k_N)$; we call this development the *kp* representation of the WMCPS. However, it is possible to study the WMCPS by using the $(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N) = qp$ representation directly. Della Riccia and Wiener (1966) and Schönberg (1952, 1953*a*,*b*) have utilized in their work the *qp* representation to discuss general aspects of the theory. In present report, our objective is to use the *qp* representation to determine an explicit solution of the Liouville equation.

The Liouville equation is a natural starting point for studies of non-equilibrium statistical mechanics (Prugovečki, 1986; Balescu, 1975). Moreover, it is known that the dynamical equation in the quantum phase space approach (Bohm and Hiley, 1981; Prugovečki, 1986; Aharanov *et al.*, 1981; Moyal, 1949) is a generalized Liouville equation, i.e., the Wigner-Moyal transform $F(Q, P, t)$ of a quantum density matrix $\rho(q', q)$ satisfies a Liouville-type equation; and in this approach the connection between quantum mechanics and Liouville's equation is made by considering the solutions of the Liouville equation as constants of the motion (Bohm and Hiley, 1981). A method to determine these solutions of the motion in the *qp* representation has been presented by Bohm and Carmi (1964*a*,*b*) in connection with a classical treatment of collective coordinates and by Bohm and Hiley (1981) in a quantum algebraic approach to generalized phase space. Unlike Bohm's method, our solution of the Liouville equation follows closely the propagator approach employed by Feynman and Hibbs (1965) in quantum theory; we show that each term of the Liouville equation propagator expanded in powers of the coupling constant can be represented uniquely by a diagram which describes a global process. In order to elucidate the method, we study the motion of an incident flow corresponding to a Maxwell distribution and we compare the results with those obtained by other authors (Prigogine, 1962).

In Section 2 we present our development and the diagrammatic technique in the *qp* representation. In Section 3 we apply this theory to the problem of Maxwell flow. In Section 4 we present our conclusions and the connection between our development and the work of Prigogine (1962).

2. PERTURBATION THEORY AND DIAGRAMMATICAL REPRESENTATION

Using the mathematical structure of HK space (Matos Neto and Vianna, 1984; Misra, 1978; Prigogine, 1980), we can write the Liouville equation as

$$i\,\partial_t|\theta_S(t)\rangle = L_S|\theta_S(t)\rangle \tag{1}$$

where $|\theta_S(t)\rangle$ is the classical state of the system whose Hermitian Liouville

operator is L_S. The subscript S signifies the classical Schrödinger picture (CSP) (Matos Neto and Vianna, 1984).

We assume that L_S can be written as $L_S = L_0 + L_1$, where L_0 is the kinematic part of L_S and L_1 contains the interaction terms. Then, in the classical interaction picture (CIP) (Matos Neto and Vianna, 1984) the vector state of the system satisfies the equation

$$|\theta(t)\rangle = U_I(t, t_0)|\theta(t_0)\rangle \tag{2}$$

with

$$i\,\partial_t U_I(t, t_0) = L_I U_I(t, t_0) \tag{3}$$

where L_I is given by $L_I = \exp[iL_0(t-t_0)]L_1 \exp[-iL_0(t-t_0)]$.

The formal solution of (3) is obtained by an iterative procedure, which gives

$$U_I(t, t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int_{t_0}^{t_1} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n\, \mathcal{T}[L_I(t_1) \cdots L_I(t_n)] \tag{4}$$

where $\mathcal{T}$ is the Wick chronological ordering operator (Matos Neto and Vianna, 1985).

In the qp representation, (2) is written as

$$\theta(\xi_1, \ldots, \xi_N, t) = \int \langle \xi_1, \ldots, \xi_N | U_I(t, t_0) | \xi_1^0, \ldots, \xi_N^0 \rangle \times \theta_0(\xi_1^0, \ldots, \xi_N^0; t_0)\, d\xi_1^0 \cdots d\xi_N^0 \tag{5}$$

The notation that we use is $\xi_j = (\mathbf{q}_j, \mathbf{p}_j)$, and $\{\xi\} = (\xi_1, \xi_2, \ldots, \xi_N) = (p; q)$ are the coordinates of an N-particle phase space. To obtain $\theta(\xi_1, \ldots, \xi_N; t)$ in (5), we use equation (4):

$$\begin{aligned}
&\theta(\xi_1, \ldots, \xi_N; t) \\
&= \int d\{\xi^0\} \langle \{\xi\} | \{\xi^0\} \rangle \theta_0(\{\xi^0\}; t_0) \\
&\quad + \int d\{\xi^0\} \sum_{n=1}^{\infty} (-1)^N \int_{t_0}^{t} t_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \langle \{\xi\} | [L_I(t_1) \\
&\quad \times L_I(t_2) \cdots L_I(t_N)] | \{\xi^0\} \rangle \theta_0(\{\xi^0\}; t_0) \\
&= \theta^{(0)}(\{\xi\}; t_0) + \sum_{n=1}^{\infty} \theta^{(n)}(\{\xi\}; t)
\end{aligned} \tag{6}$$

We compute each term in (6):

For $n=0$

$$\theta^{(0)}(p, q; t)$$
$$= \int dp_1\, dp_2 \cdots dp_N\, dq_1 \cdots dq_N\, \delta(p_1 - p_1^0)\, \delta(p_2 - p_2^0)$$
$$\times \cdots \times \delta(p_N - p_N^0)\, \delta(q_1 - q_1^0) \times \cdots \times \delta(q_N - q^0)\theta_0(q_1^0 \cdots p_N^0; t_0)$$
$$= \theta_0(p, q; t_0) \tag{7}$$

For $n=1$

$$\theta^{(1)} = -\int_{t_0}^{t} dt_1\, F(\tau_{10})\Gamma_{10}\theta_0(p, q; t_0) = S_1\theta_0(p, q; t_o) \tag{8}$$

where we used

$$-i\langle pq|L_I|p'q'\rangle = \delta(q-q')\, \delta(p-p')\, F(q', p')\, \nabla_p$$
$$F(q, p)\nabla_p = -\frac{\partial H}{\partial q}\nabla_p = -\sum_{i=1}^{N} \frac{\partial H}{\partial \mathbf{q}_i}\frac{\partial}{\partial \mathbf{p}_i}$$

H is the Hamiltonian, $\tau_{ab} = t_a - t_b$, and

$$F(\tau_{ab}) = F\left(q, \frac{\mathbf{p}}{m}\tau_{ab}; p\right)$$
$$= F\left(\mathbf{q}_1 + \frac{\mathbf{p}_1}{m}\tau_{ab}, \mathbf{q}_2 + \frac{\mathbf{p}_2}{m}\tau_{ab}, \ldots, \mathbf{q}_N + \frac{\mathbf{p}_N}{m}\tau_{ab}; \mathbf{p}_1, \ldots, \mathbf{p}_N\right) \tag{9}$$

The operator $\Gamma_{ab} = \nabla_p - (\tau_{ab}/m)\, \nabla_q$ is such that ∇_p acts on the function in phase space with explicit p dependence.

For $n=2$

$$\theta^{(2)} = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \{F(\tau_{10})F(\tau_{20})\Gamma_{10}\Gamma_{20}$$
$$+ F(\tau_{10})[\Gamma_{12}F(\tau_{20})]\}\theta_0(q, p; t_0)$$
$$= S_2\theta_0(q, p; t_0) \tag{10}$$

and so on.

For any value of n we can write

$$\theta^{(n)}(q, p; t) = S_n\theta_0(q, p; t_0) \tag{11}$$

so that

$$\theta(q, p; t) = S\theta_0(q, p; t_0) = \sum_{n=0}^{\infty} S_n\theta_0(q, p; t_0) \tag{12}$$

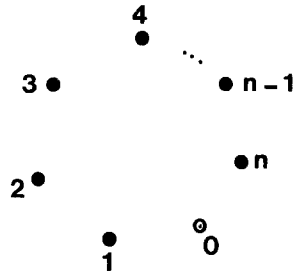

Fig. 1

Obviously, S_0, S_1, and S_n are known from equations (7), (9), and (10). The generic term S_n is given by

$$S_n = (-1)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_n} dt_n \left\{ \sum_{r_1 \cdots r_n = 0}^{n\,\prime} \left(\prod_{s=1}^{n} \Gamma_{sr_s} \right) \prod_{s=1}^{n} F(\tau_{s0}) \right. \quad (13)$$

The prime in the summation symbol means that $s \neq 0$; $s > r$. The operators Γ_{rs} in (13) have the following properties (p):

p-1: $r \neq s$ for any $r, s \in (0, 1, 2, \ldots, n)$.

p-2: $\max(r) = n$, $\max(s) = n$; $\min(r) = 0$, $\min(s) = 1$; where $\max(t)$ and $\min(t)$ mean maximum and minimum value, respectively, for t.

p-3: when $s < r$, Γ_{sr} operates on the functions $F(\tau_{r0})$; when $s > r$, $\Gamma_{sr} \equiv \Gamma_{s0}$ and Γ_{s0} operates on the functions θ_0 only when the operation $\theta(q, p; t) = S_n \theta_0(q, p; t_0)$ had been performed.

p-4: $[\Gamma_{sr}, \Gamma_{s'r'}]_- = \Gamma_{sr}\Gamma_{s'r'} - \Gamma_{s'r'}\Gamma_{sr} = 0$.

Owing to these properties, we are able to obtain a diagrammatic representation for the term S_n. Thus, we have the following rules (r) to compose the diagrams:

r-1: For the nth term we enumerate the $n+1$ vertex of a regular polygon from 0 to n in the clockwise direction (Figure 1).

r-2: Each vertex is connected to another by an orientated line representing an operator Γ_{sr} (Figure 2).

r-3: Only one line leaves a vertex, but there is no limitation to the number of lines entering a vertex.

Fig. 2

r-4: A line leaving vertex s can enter a vertex 0 or another vertex $r \neq 0$, with $r > s$.

r-5: No line leaves the vertex zero (receptor, vertex), which we represent by $\odot$. The other vertex we will represent by $\bullet$.

r-6: There are $n!$ different ways to connect $n+1$ given vertexes such that one line leaves each vertex. Each one of these ways represents in the integral in equation (13) a term of the form

$$\Gamma_{1r_1}\Gamma_{2r_2}\cdots\Gamma_{nr_n}$$

We calculate, as examples, the terms S_2 and S_3 which will be used in the application.

For $n=2$ (see Figure 3)

$$S_2 = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \,[\Gamma_{10}\Gamma_{20}+\Gamma_{20}\Gamma_{12}]F(\tau_{10})F(\tau_{20}) \tag{14}$$

From equation (14) and properties (p-1) to (p-4) we obtain equation (10).

For $n=3$ (see Figure 4)

$$S_3 = (-1)\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 \,[\Gamma_{10}\Gamma_{20}\Gamma_{30}+\Gamma_{12}\Gamma_{23}\Gamma_{30}+\Gamma_{10}\Gamma_{23}\Gamma_{30}$$
$$+\Gamma_{12}\Gamma_{20}\Gamma_{30}+\Gamma_{13}\Gamma_{23}\Gamma_{30}+\Gamma_{12}\Gamma_{30}\Gamma_{20}]F(\tau_{10})F(\tau_{20})F(\tau_{30}) \tag{15}$$

We remark that by consistency the vertex n is always connected to the receptor vertex.

The diagrams that we introduce are interpreted in terms of the whole process. Indeed, we observe that the diagrams, in accordance with rules r-1 and r-2, are such that each line represents an operator Γ_{sr}. These Γ_{sr} are N-particle operators. The operators Γ_{s0} modify the wave functions $\theta_0(q, p; t_0)$, and Γ_{sr} $(s \neq r \neq 0)$ change the interaction term $F(\tau_{r0})$, among the particles.

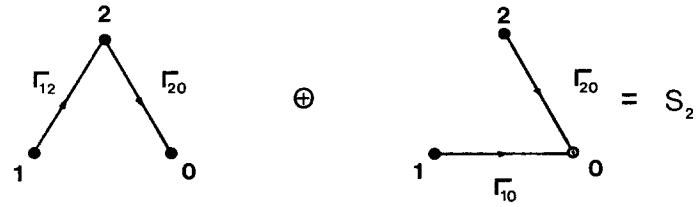

Fig. 3

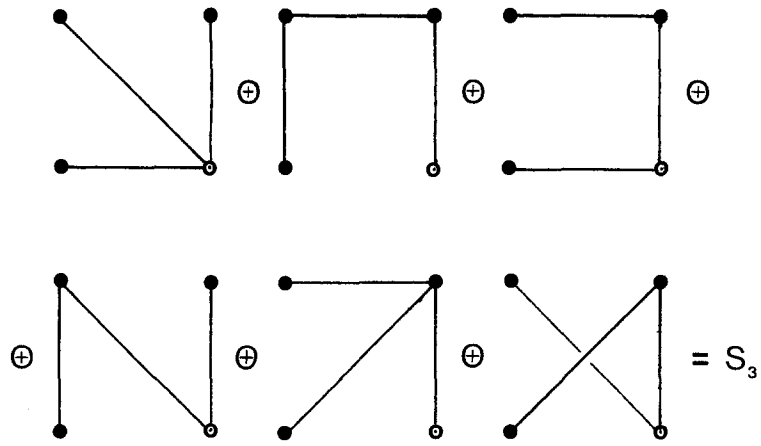

Fig. 4

3. SCATTERED PARTICLE BY A POTENTIAL $\lambda V(q)$

As an application of our method, we study a particle scattered by a potential $\lambda V(q)$. For the sake of simplicity, we consider here only the one-dimensional case. Let the initial state be

$$\theta_0(p, t_0) = \theta_M(p, t_0 = 0) = A\, e^{-\beta p^2/2}$$

which gives the Maxwell velocity distribution when we calculate $|\theta|^2$, where we have used $m = 1$, $A = (\pi kT/2)^{1/4}$, and $\beta = 1/k_B T$. Thus we obtain for the first terms of the expansion (13):

For $n = 0$

$$\theta^{(0)} = \theta_M(p) \tag{16}$$

For $n = 1$

$$\begin{aligned}\theta^{(1)} &= -\int_0^t dt_1\, F(\tau_{10})\Gamma_{10}\theta_M(p) \\ &= -\lambda A\beta[V(q+pt) - V(q)]\, e^{-\beta p^2/2}\end{aligned} \tag{17}$$

For $n = 2$

$$\begin{aligned}\theta^{(2)} = {} & \tfrac{1}{2}A\lambda^2\beta^2 V^2(q)\, e^{-\beta p^2/2} + A\lambda^2\beta^2 V(q+pt)\, e^{-\beta p^2/2} \\ & + A\lambda^2\beta^2 V(q)\, V(q+pt)\, e^{-\beta p^2/2} \\ & - A\lambda^2\beta[\nabla_q V(q)]\left[tV(q+pt) - \int_0^t dt_1\, V(q+pt_1)\right] e^{-\beta p^2/2}\end{aligned} \tag{18}$$

For $n=3$

$$\theta^{(3)}=\Bigg(-\beta A\lambda^3\frac{1}{3!}V^3(q+pt)-\beta^3A\lambda^3\Bigg[-\frac{1}{3!}V^3(q)$$
$$+\frac{1}{2}V^2(q)V(q+pt)-\frac{1}{2}V(q)V^2(q+pt\Bigg]$$
$$-\beta pA\lambda^3\Bigg\{-\frac{1}{p^4}[\nabla_q V(q)]V^2(q+pt)t$$
$$+\frac{1}{p^4}[\nabla_q V(q)]\int_0^t dt_1\,V^2(q+pt_1)$$
$$+\frac{2}{p^4}[\nabla_q V(q)]\int_0^t dt_1\frac{d}{dt_1}V(q+pt_1)\int_0^{t_1}dt_2\,V(q+pt_2)\Bigg\}$$
$$-A\lambda^3\beta^2p^2\Bigg\{-\frac{1}{2p^3}[\nabla_q V(q)]V^2(q+pt)t$$
$$+\frac{1}{2p^3}[\nabla_q V(q)]\int_0^t dt_1\,V^2(q+pt_1)$$
$$+\frac{1}{p^3}[\nabla_q V(q)]\int_0^t dt_1\frac{d}{dt_1}V(q+pt_1)\int_0^{t_1}dt_2\,V(q+pt_2)\Bigg\}$$
$$-A\beta p\lambda^2\Bigg\{-\frac{1}{2p^3}[\nabla_q^2 V(q)]V^2(q+pt)t^2$$
$$+\frac{1}{p^3}[\nabla_q^2 V(q)]\int_0^t dt_1\,V^2(q+pt_1)t_1+\frac{1}{p^3}[\nabla_q^2 V(q)]$$
$$\times\int_0^t dt\,t_1\frac{d}{dt_1}V(q+pt_1)\int_0^{t_1}dt_2\,V(q+pt_2)\Bigg\}$$
$$-A\lambda^3(-\beta+\beta^2p^2)\Bigg\{\frac{1}{p^3}V(q)[\nabla_q V(q)]V(q+pt)t$$
$$-\frac{1}{p^3}V(q)[\nabla_q V(q)]\int_0^t dt_1\,V(q+pt_1)\Bigg\}\Bigg)e^{-\beta p^2/2} \tag{19}$$

We suppose that the potential $V(q)$ is a sufficiently smooth function in order to give to expression (13) a mathematical meaning.

When $V(q)$ is a short-range potential, such that $\lim_{t\to\infty}V(q-pt)\to 0$, we can calculate the asymptotic state $\lim_{t\to\infty}\theta_S(q,p;t)$. In this case, from our expressions (16)–(19), it follows that in CPS we obtain

$$\theta_S(q,p,t\to\infty)=\theta_{MB}(q,p)=A\,e^{-\beta[p^2/2+\lambda V(q)]}$$

We have, therefore, that the system is a nonstationary state after the collision, but evolves to a stationary state in the asymptotic limit. This conclusion is the starting point for the dynamical derivation of equilibrium statistical mechanics using a long-time interaction effect on the Maxwell equilibrium distribution in the method developed by Prigogine and co-workers (Prigogine, 1962).

4. CONCLUDING REMARKS

In this report we have presented a perturbative method in classical phase space in order to obtain a solution of the Liouville equation. Our method uses the fact that the classical Liouville equation can be formulated as a dynamical equation in Hilbert-Koopman space. In consequence, our development can be applied also to Liouville-type equations derived in the quantum phase approach (Bohm and Hiley, 1981; Prugovečk, 1986).

We have used the *qp* representation. Nevertheless, we can transform our solution to other representations of the HK space and in particular to the *kp* representation. In this sense, the dynamic of correlations (Prigogine, 1962; Balescu 1975) can be derived directly from our approach. Indeed, using $|kp\rangle = |k_1, k_2, \ldots, k_N, p_1 \cdots p_N\rangle$, so that $\langle kp|\theta(t)\rangle = \rho_k(p; t)$, we obtain from equation (2)

$$\rho_k(p; t) = \langle kp| U_1 |\theta_0(t_0)\rangle \tag{20}$$

Using a complete set of eigenkets $\{|kp\rangle\}$, it is an easy matter to show that (20) coincides with the result derived by the correlation dynamics theory when one chooses as solution of (1) L-integrable real-valued functions. We note, however, that each diagram in the *qp* representation corresponds to several diagrams in the *kp* representation.

As a final remark, we note that by our method we have obtained the complete solution of the Maxwell flow problem, i.e., the vector state $|\theta(t)\rangle$ at any time, and showed that its asymptotic value coincides with that obtained by Prigogine (1962) using an approximate master equation for ρ_k.

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