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Brownian motion, quantum corrections and a generalization of the Hermite polynomials

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ABSTRACT

The nonequilibrium evolution of a Brownian particle, in the presence of a "heat bath" at thermal equilibrium (without imposing any friction mechanism from the outset), is considered. Using a suitable family of orthogonal polynomials, moments of the nonequilibrium probability distribution for the Brownian particle are introduced, which fulfill a recurrence relation. We review the case of classical Brownian motion, in which the orthogonal polynomials are the Hermite ones and the recurrence relation is a three-term one. After having performed a long-time approximation in the recurrence relation, the approximate nonequilibrium theory yields irreversible evolution of the Brownian particle towards thermal equilibrium with the "heat bath". For quantum Brownian motion, which is the main subject of the present work, we restrict ourselves to include the first quantum correction: this leads us to introduce a new family of orthogonal polynomials which generalize the Hermite ones. Some general properties of the new family are established. The recurrence relation for the new moments of the nonequilibrium distribution, including the first quantum correction, turns out to be also a three-term one, which justifies the new family of polynomials. A long-time approximation on the new three-term recurrence relation describes irreversible evolution towards equilibrium for the new moment of lowest order. The standard Smoluchowski equations for the lowest order moments are recovered consistently, both classically and quantum-mechanically.

1. Introduction

We shall consider a "heat bath", at complete thermal equilibrium at absolute temperature T. We shall treat the nonequilibrium statistical mechanics of a Brownian particle of mass m in one spatial dimension x, in the presence of the "heat bath" and subject to a real time-independent potential $V(=V(x))$. By assumption, the particle is not at thermal equilibrium with the "heat bath" at the initial time $t = 0$. We shall concentrate on the time evolution of the particle for $t > 0$, both in the classical regime and not far from the latter, including the first quantum correction.

Let us recall classical Brownian motion, as described by the irreversible Kramers equation [1]. The latter follows by assuming either some model for the interaction between the "heat bath" and the particle, or some friction mechanism on the latter, from the outset. By using suitable Hermite polynomials in the particle momentum (which are orthogonalized with respect to the equilibrium Boltzmann distribution), moments of the nonequilibrium probability distribution have been introduced [2]. Those moments fulfill a three-term recurrence relation (or hierarchy) [2], to which various techniques

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can be applied [3,4]. On the other hand, for classical closed large systems (without a "heat bath"), a suitable long-time approximation has been imposed on the three-term hierarchy for the reversible Liouville equation [5,6]: then, the resulting approximate nonequilibrium theory for the moments yields irreversible behavior towards thermal equilibrium consistently. The same also holds for a classical Brownian particle in the presence of a "heat bath" [6], without assuming (ab initio) friction effects on the particle: see Section 2 below.

The generalizations for quantum Brownian motion are more difficult. For those including friction, see, for instance, [7–9] and references therein. For other related research, see [10–18] and references therein. In [8,9], the quantum particle is described by the Wigner distribution function [19,20] including friction from the outset, and one employs Hermite polynomials in the particle momentum, similar to those for the classical case, in order to define the nonequilibrium moments. Then, the recurrence relation or hierarchy satisfied by the moments is not a three-term one, due to quantum corrections, which complicates the analysis rather considerably [8,9]. We shall deal with quantum Brownian motion by including only the first quantum correction. We shall not assume (ab initio) friction effects on the particle. Then, we shall study possible definitions of new moments, which could lead to three-term recurrence relations, in which the methods of [5,6] could be employed (at least, in some simple version), so as to have approximate irreversibility for long time. In turn, the search for those new moments will require the introduction of a new and suitable family of orthogonal polynomials.

This work is organized as follows. Section 2 summarizes the nonequilibrium statistical mechanics of the classical Brownian particle using the classical Liouville distribution function, the moments of the latter by means of the Hermite polynomials and the approximate long-time theory and irreversible behavior for the moments [5,6]. Section 3 reminds the nonequilibrium statistical mechanics of the quantum Brownian particle, using the Wigner distribution function, the equilibrium Wigner function and the first quantum corrections [19,20], which distinguish the latter from the classical Liouville distribution function. Section 4 introduces a new family of orthogonal polynomials, $H_{x,2,n}$, determined by the equilibrium Wigner function with first quantum corrections. In Section 5, the dynamical equation for the Wigner distribution function is transformed, using the $H_{x,2,n}$'s, into a three-term recurrence relation which, in turn, is subject to suitable long-time approximations. Section 6 contains conclusions and discussions.

2. Classical Brownian particle

Let the classical particle have momentum p and Hamiltonian

$$H = p^2/(2m) + V \tag{1}$$

$V = V(x)$ being a real potential. From the outset, we shall not suppose any friction effects on the particle. The classical (c) probability distribution $W_c = W_c(x, p; t)$ for the particle fulfills the reversible Liouville equation:

$$\frac{\partial W_c}{\partial t} = \{H, W_c\} = -\frac{p}{m}\frac{\partial W_c}{\partial x} + \frac{\mathrm{d}V}{\mathrm{d}x}\frac{\partial W_c}{\partial p} \tag{2}$$

$\{H, W_c\}$ stands for the classical Poisson bracket. The initial condition at $t = 0$ is $W_{c,in}$.

Any integration will be performed in $(-\infty, +\infty)$. We shall introduce the following moments $W_{c,n}$ ($n = 0, 1, 2, \ldots$) of W_c regarding the p-dependence [2–6]:

$$W_{c,n} = W_{c,n}(x; t) = \int \mathrm{d}p \frac{H_n(p/q_{eq})}{(\pi^{1/2} 2^n n!)^{1/2}} W_c \tag{3}$$

$$q_{eq} = (2m/\beta)^{1/2}, \quad \beta = \frac{1}{K_{\mathrm{B}}T} \tag{4}$$

which incorporate the equilibrium temperature T of the "heat bath". H_n is the Hermite polynomial of order n [21]. K_{B} is Boltzmann's constant. Eq. (3) and (2) imply the following infinite reversible three-term linear recurrence relation for all $W_{c,n}$'s ($n = 0, 1, 2, \ldots, W_{c,-1} = 0$) [2–6]:

$$\frac{\partial W_{c,n}}{\partial t} = -M_{c;n,n+1} W_{c,n+1} - M_{c;n,n-1} W_{c,n-1} \tag{5}$$

$$M_{c;n,n+1} W_{c,n+1} \equiv \left[\frac{(n+1)}{m\beta}\right]^{1/2} \frac{\partial W_{c,n+1}}{\partial x} \tag{6}$$

$$M_{c;n,n-1} W_{c,n-1} \equiv \left[\frac{n}{m\beta}\right]^{1/2} \left(\frac{\partial W_{c,n-1}}{\partial x} + \beta \frac{\mathrm{d}V}{\mathrm{d}x} W_{c,n-1}\right). \tag{7}$$

The initial condition $W_{c,in,n}$ for Eq. (5) is obtained by replacing W_c by $W_{c,in}$ in (3). A t-independent solution of Eq. (2) is:

$$W_{c,eq} = W_{c,eq}(x,p) = \exp\left[-\beta\left(\frac{p^2}{2m} + V(x)\right)\right] \quad (8)$$

$W_{c,eq}$ yields, through (3), moments $W_{c,eq,0}$ proportional to $\exp[-\beta V]$ and $W_{c,eq,n} = 0$, $n > 0$.

We introduce the Laplace transform:

$$\tilde{W}_{c,n}(s) \equiv \int_0^{+\infty} \mathrm{d}t W_{c,n} \exp(-st). \quad (9)$$

One difficulty with (5) and with its Laplace transform for the $\tilde{W}_{c,n}(s)$'s is the absence of an explicit relationship between $M_{c;n,n+1}$ and $M_{c;n,n-1}$, for $V \neq 0$. To solve that difficulty, we introduce $g_n = g_n(s) \equiv W_{c,eq,0}^{-1/2}\tilde{W}_{c,n}(s)$. Then, (5) and (9) yield the new hierarchy:

$$sg_n = W_{c,eq,0}^{-1/2} W_{c,in,n} - M'_{c;n,n+1} g_{n+1} - M'_{c;n,n-1} g_{n-1} \quad (10)$$

$$M'_{c;n,n+1} g_{n+1} \equiv \left[\frac{(n+1)}{m\beta}\right]^{1/2} \left(\frac{\partial g_{n+1}}{\partial x} - \frac{\beta}{2}\frac{\mathrm{d}V}{\mathrm{d}x} g_{n+1}\right) \quad (11)$$

$$M'_{c;n,n-1} g_{n-1} \equiv \left[\frac{n}{m\beta}\right]^{1/2} \left(\frac{\partial g_{n-1}}{\partial x} + \frac{\beta}{2}\frac{\mathrm{d}V}{\mathrm{d}x} g_{n-1}\right). \quad (12)$$

Notice that a relationship now exists between $M'_{c;n,n+1}$ and $M'_{c;n,n-1}$: $M'_{c;n,n+1}$ is the adjoint of $-M'_{c;n,n-1}$, for any V. The hierarchy (10) can be solved formally by applying to it standard procedures for solving numerical three-term linear recurrence relations in terms of continued fractions (see, for instance, [3,4]). Thus, one neglects $g_{n'+1}(s)$ in (10) for given n', solves for $g_{n'}(s)$ in terms of $g_{n'-1}(s)$, proceeds to (10) for $n'-1$, solves for $g_{n'-1}(s)$ in terms of $g_{n'-2}(s)$ and so on. Then, one infers directly the general formal (continued-fraction) structure of the solution as $n' \to +\infty$. That formal procedure yields all $g_n(s)$, for any $n = 1, \ldots$, in terms of sums of products of certain s-dependent linear operators $D[n'; s]$, $n' \geq n$, acting upon $g_{n-1}(s)$ and upon all $W_{c,eq,0}^{-1/2} W_{c,in,n'}$'s, with $n' \geq n$. The linear operators $D[n; s]$'s are defined recurrently through:

$$D[n; s] = [s - M'_{c;n,n+1} D[n+1; s] M'_{c;n+1,n}]^{-1}. \quad (13)$$

The successive iterations of (13) generate an infinite continued fraction of operators. The solution for $g_n(s)$ is only formal up to this stage, because the M' are linear operators and, hence, the $D[n; s]$'s are infinite continued fractions of products of the linear operators M'. Thus, once the formal solution has been obtained, one should try to give a less formal and more precise meaning to it. This has been done succinctly in [5] for $V = 0$ (by performing Fourier transforms in x). Compact expressions for the linear operators D's, as finite fractions, have been given also succinctly in [6], when V represents a harmonic oscillator potential. See [3,4] for reductions of the D's (using further expansions into orthonormal basis, regarding x-dependences) to matrix continued fractions, to be subject later to numerical computations in various cases. For our purposes, the following outline should suffice in order to give a somewhat more precise characterization of (10) and of (13): see [5,6] for other presentations and details. The fact that $M'_{c;n,n+1}$ is the adjoint of $-M'_{c;n,n-1}$ and the structure of (13) imply the following crucial properties for suitably fixed real $\epsilon > 0$ [5,6]: (i) if $D[n+1; \epsilon]$ were Hermitian and if all its eigenvalues (which would be real) were non-negative, then the same would hold true for $D[n; \epsilon]$, and (ii) through iterative arguments, hermiticity and impossibility of negative eigenvalues appear to hold true for the successive $D[n; \epsilon]$'s.

Thus far, no long-time approximation has been performed. We shall analyze the approximate irreversible evolution of the classical Brownian particle towards thermal equilibrium with the "heat bath". We choose some $n_0(\geq 1)$ and, for $n \geq n_0$, set $s = \epsilon > 0$ in any $D[n; s]$, ϵ being suitably small. Then, the long-time approximation for $n \geq n_0$ reads: we replace any $D[n'; s]$ yielding $g_n(s)$, $n \geq n_0$, in terms of $g_{n-1}(s)$ and of $W_{c,eq,0}^{-1/2} W_{c,in,n''}$'s, $n'' \geq n$, by $D[n'; \epsilon]$. That approximation is not done for $n < n_0$, and it is the better fulfilled the larger n_0 is. For a simpler analysis, we also neglect all $W_{c,eq,0}^{-1/2} W_{c,in,n'}$'s for any $n' \geq n_0$. Then, the general solution for $g_{n_0}(s)$ provided by the formal procedure outlined above, becomes approximately, for small s (say, long time):

$$g_{n_0}(s) \simeq -D[n_0; \epsilon] M'_{c;n_0,n_0-1} g_{n_0-1}(s). \quad (14)$$

By using Eq. (5), as they stand, for $n = 0, 1, ., n_0 - 1$, and the inverse Laplace transform of (14) (recast back in terms of $\tilde{W}_{c,n_0}(s)$ and $\tilde{W}_{c,n_0-1}(s)$) the hierarchy becomes closed for $W_{c,n}$, $n_0 = 0, 1, ., n_0 - 1$. The t-independent solution of the closed approximate hierarchy is $W_{c,eq,0}$ and $W_{c,eq,n} = 0$, $n = 1, 2, \ldots, n_0 - 1$. The solutions of the closed approximate hierarchy relax irreversibly, for $t \gg 0$ and any reasonable $W_{c,in}$, towards the above t-independent solution: the classical Brownian particle evolves towards thermal equilibrium with the "heat bath" [5,6]. We still require a procedure for computing $D[n_0; \epsilon]$ or an ansatz for it.

In the simplest case, $n_0 = 1$, we approximate the linear operator $D[1; \epsilon]$ by a real constant $\gamma^{-1}m(>0)$. $\gamma^{-1}m$ tries to approximate somehow, on the average, the set of all eigenvalues (all being real and non-negative) of the linear operator $D[1; \epsilon]$. This ansatz for $D[1; \epsilon]$ is a practical simplification, which supplements the above long-time approximation. Then, we combine (14) for $n_0 = 1$ and (5) for $n = 0$. The resulting (irreversible) equation for the $n = 0$ moment $W_{c,0}$ of the classical probability distribution W_c is the Smoluchowski one:

$$\frac{\partial W_{c,0}}{\partial t} = \frac{1}{\beta\gamma}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} + \beta\frac{dV}{dx}\right]W_{c,0} \tag{15}$$

with the initial condition $W_{c,in,0}$ at $t = 0$. The moment procedure and the long-time approximations in [5,6], without having assumed friction effects from the outset, lead to the Smoluchowski equation in (15), which is identical to those obtained by other authors through very different procedures [4,22] (involving ab initio friction). Thus, the positive constant γ in (15) plays the same role as the friction coefficient in the standard derivations [4,22].

3. Quantum Brownian particle: Background

3.1. Nonequilibrium Wigner function

We shall now consider a quantum Brownian particle of mass m and momentum operator $-i\hbar(\partial/\partial x)$, in one spatial dimension x, with quantum Hamiltonian:

$$H_Q = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \tag{16}$$

$\hbar$ being Planck's constant, and $V = V(x)$ being also a real potential. We shall outline the nonequilibrium quantum statistical mechanics of the particle in the presence of the "heat bath". The time evolution for $t > 0$ of the particle is given by the density operator $\rho = \rho(t, 0)$ (a statistical mixture of states). In the actual quantum case, we shall not suppose any ab initio friction effects on the particle either. The density operator fulfills the reversible Dirac-von Neumann equation:

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}[H_Q, \rho] = \frac{1}{i\hbar}(H_Q\rho - \rho H_Q) \tag{17}$$

with the initial condition $\rho(0, 0) = \rho_{in}$. $[H_Q, \rho]$ denotes the commutator. We consider the matrix element $\langle x - y|\rho(t, 0)$ $|x + y\rangle$ of $\rho(t, 0)$ in generic eigenstates, $|x - y\rangle$, $|x + y\rangle$, of the quantum position operator. Any integration will be performed in $(-\infty, +\infty)$. The quantum Wigner distribution function $W = W(x, q; t)$, determined by ρ, is [19,20]:

$$W(x, q; t) = \frac{1}{\pi\hbar}\int dy \exp\left[\frac{i2qy}{\hbar}\right]\langle x - y|\rho(t, 0)|x + y\rangle. \tag{18}$$

The reversible dynamical evolution of W is given by [19,20]:

$$\frac{\partial W(x, q; t)}{\partial t} = -\frac{q}{m}\frac{\partial W(x, q; t)}{\partial x} + \int dq' W(x, q + q'; t)\left[\frac{i}{\pi\hbar^2}\right]\int dy[V(x + y) - V(x - y)]\exp\left[-\frac{i2q'y}{\hbar}\right]. \tag{19}$$

The right-hand-side of the quantum evolution equation (19) gives rise, upon expanding suitably $V(x + y) - V(x - y)$, to additive corrections of order $\hbar^2$ and higher [19]. Corrections of order $\hbar$ vanish exactly, in general. It is well known that $W(x, q; t)$ could take on negative values in some regions, in principle.

3.2. Equilibrium Wigner function W_{eq}

Let the quantum particle be at thermal equilibrium, at temperature T, with the "heat bath". Recalling Eq. (4), the equilibrium density operator is $\rho_{eq} = \exp[-\beta H_Q]$ which, through Eq. (18), determines the equilibrium (t-independent) Wigner function $W_{eq} = W_{eq}(x, q)$. There seems to be no known compact expression for W_{eq} for any V and any β. For high temperature T (small β) and small $\hbar$ (not far from the classical, $\hbar \to 0$, limit), a systematic expansion for W_{eq} for a general V, as a power series in $\hbar^2$, exists [19,20] (all contributions in odd powers of $\hbar$ vanish identically). We shall quote [19,20]:

$$W_{eq}(x, q) \simeq W_{eq,2}(x, q) = W_{c,eq}\left[1 + \hbar^2\left[-\frac{\beta^2}{8m}\frac{d^2V}{dx^2} + \frac{\beta^3}{24m}\left(\frac{dV}{dx}\right)^2 + \frac{\beta^3 q^2}{24m^2}\frac{d^2V}{dx^2}\right]\right] \tag{20}$$

$W_{c,eq}$ is given in (8), with $p = q$. The subscript 2 reminds that $W_{eq,2}(x, q)$ includes the full contributions up to and including order $\hbar^2$, but all contributions of orders $\hbar^{2n''}$, $n'' \geq 2$ are disregarded. $W_{c,eq}$ is the classical Liouville probability distribution for thermal equilibrium. For the one dimensional case, the full contribution of order $\hbar^4$ to $W_{eq}(x, q)$ has also been computed in [19].

4. Orthogonal polynomials $H_{x,2,n}(q/q_{eq})$ for $W_{eq,2}$

4.1. Construction of $H_{x,2,n}(q/q_{eq})$

It seems natural to rewrite $W_{eq,2}(x,q)$, up to and including order $\hbar^2$ [19], in terms of the Hermite polynomials H_{2n} [21], $n = 0, 1$:

$$W_{eq,2}(x,q) = W_{c,eq} \sum_{n=0}^{1} a_{2n}(x) H_{2n}(q/q_{eq}). \tag{21}$$

In turn, the coefficients $a_{2n}(x)$ are polynomials of second order in $\hbar^2$, which depend on first and second derivatives of $V(x)$ and on β. One has:

$$a_0(x) = 1 + \frac{\hbar^2}{8}\left[\frac{\beta^3}{3m}\left(\frac{\mathrm{d}V}{\mathrm{d}x}\right)^2 - \frac{2\beta^2}{3m}\frac{\mathrm{d}^2V}{\mathrm{d}x^2}\right] \tag{22}$$

$$a_2(x) = \frac{\beta^2\,\hbar^2}{48m}\frac{\mathrm{d}^2V}{\mathrm{d}x^2}. \tag{23}$$

We cannot warrant that $W_{eq}(x,q)$ be non-negative in some regions in general. However, for small β and $\hbar$ (not far from the classical limit), Eq. (20) indicates that $W_{eq,2}(x,q)$, up to and including order $\hbar^2$, could be non-negative for any x and q, provided that first and second derivatives of $V(x)$ remain bounded in absolute value. We shall suppose this non-negativity of $W_{eq,2}(x,q)$ in what follows. As we shall see, it will be interesting to introduce the denumerably infinite family of all polynomials in q, $H_{x,2,n}(q/q_{eq})$ (a kind of generalization of the Hermite polynomials), $n = 0, 1, 2, 3, \ldots$, with the following properties:

(1) $H_{x,2,n}(q/q_{eq})$ equals $H_n(q/q_{eq})$ (say, without any multiplicative factor depending on β, $\hbar$ or x) plus a remainder of order $\hbar^2$, which is another polynomial in q and also depends on β and x: see below. Hence, $H_{x,2,n}(q/q_{eq})$ contains no contribution of order $\hbar^{n''}$, $n'' \geq 4$. Thus, $H_{x,2,n}(q/q_{eq})$ depends parametrically on x, as indicated by the subscript, and also on β and on $\hbar$, but the latter two dependences will not be explicited. The subscript 2 reminds that $H_{x,2,n}(q/q_{eq})$ includes up to order $\hbar^2$, but all orders $\hbar^{2n''}$, $n'' \geq 2$ are excluded.

(2) Provided that we integrate in $-\infty < q < +\infty$ with the weight function $W_{eq,2}(x,q)$ given by (21), leaving x unintegrated, the $H_{x,2,n}(q/q_{eq})$'s constitute a denumerably infinite orthogonal set, up to and including order $\hbar^2$. Then, for $n \neq n'$ and any x, we impose that:

$$\int \mathrm{d}q W_{eq,2}(x,q) H_{x,2,n}(q/q_{eq}) H_{x,2,n'}(q/q_{eq}) = 0 \tag{24}$$

holds up to and including order $\hbar^2$, but contributions of order $\hbar^{2n''}$, $n'' \geq 2$ are disregarded.

One has, trivially:

$$H_{x,2,0}(q/q_{eq}) = 1 = H_0(q/q_{eq}) \tag{25}$$

$$H_{x,2,1}(q/q_{eq}) = \frac{2q}{q_{eq}} = H_1(q/q_{eq}). \tag{26}$$

The determination of $H_{x,2,n}(q/q_{eq})$, for $n \geq 2$ will be facilitated by the following integral:

$$\int \mathrm{d}y \exp(-x^2) H_2(y) H_n(y) H_l(y) = 2(\pi 2^{n+l} n! l!)^{1/2} [((n+1)(n+2))^{1/2}\delta_{l,n+2} + 2n\delta_{l,n} + (n(n-1))^{1/2}\delta_{l,n-2}] \tag{27}$$

which can be derived from Eqs. [A.55] and [A.58] in [23]. $\delta_{l,n}$ is the Kronecker delta. We search for $H_{x,2,n}(q/q_{eq})$, $n \geq 2$, as

$$H_{x,2,n}(q/q_{eq}) = H_n(q/q_{eq}) - b_n(x) H_{n-2}(q/q_{eq}). \tag{28}$$

The unknown function $b_n(x)$, $n \geq 2$, is to be determined from:

$$\int \mathrm{d}q W_{eq,2}(x,q) H_{x,2,n}(q/q_{eq}) H_{x,2,n-2}(q/q_{eq}) = 0 \tag{29}$$

disregarding contributions of order $\hbar^{n''}$, $n'' \geq 3$. One finds easily:

$$b_n(x) = 4n(n-1) a_2(x). \tag{30}$$

4.2. Properties of $H_{x,2,n}(q/q_{eq})$

The $H_{x,2,n}(q/q_{eq})$'s are not normalized with respect to the measure $\int dq W_{eq,2}(x,q)$. The orthonormalized polynomials are $H_{x,2,n}(q/q_{eq})/N_n(x)$, with:

$$N_n(x) \equiv \left[\int dq W_{eq,2}(x,q) H_{x,2,n}(q/q_{eq})^2\right]^{1/2}. \tag{31}$$

One finds (disregarding contributions of order $\hbar^{n''}$, $n'' \geq 3$):

$$N_n(x) = \exp[-2^{-1}\beta V(x)] q_{eq}^{1/2} (\pi^{1/2} n! 2^n)^{1/2} \left[1 + \frac{\hbar^2}{16}\left(\frac{\beta^3}{3m}\left(\frac{dV}{dx}\right)^2 - \frac{2\beta^2}{3m}\frac{d^2V}{dx^2}\right) + 2na_2(x)\right]. \tag{32}$$

The $H_{x,2,n}(q/q_{eq})$'s fulfill the following recurrence relations (again, up to and including order $\hbar^2$ and disregarding contributions of order $\hbar^{n''}$, $n'' \geq 3$), with $H_{x,2,-1} \equiv 0$:

$$\frac{dH_{x,2,n}(y)}{dy} = 2nH_{x,2,n-1}(y) \tag{33}$$

$$2yH_{x,2,n}(y) = H_{x,2,n+1}(y) + 2n(1 + 4a_2(x))H_{x,2,n-1}(y). \tag{34}$$

The $H_{x,2,n}(q/q_{eq})$'s have the following generating function (z being a real parameter):

$$\left[1 - a_2(x)\frac{\partial^2}{\partial y^2}\right]\exp[-z^2 + 2zy] = \sum_{n=0}^{+\infty} \frac{z^n}{n!} H_{x,2,n}(y). \tag{35}$$

Recall that the x-dependence of $V(x)$ is quite general. Then, we shall comment about the x-dependences in Eq. (35): that of $a_2(x)$ in its left-hand-side matches exactly the one in its right-hand-side, from all polynomials $H_{x,2,n}(y)$ (through all $-b_n(x)$'s: recall Eqs. (28) and (30)).

We recall that other generalizations of the Hermite polynomials exist in the literature about orthogonal polynomials: for instance, the one in [24]. Those generalizations are different (and have different motivations) from the $H_{x,2,n}(q/q_{eq})$'s (which arise from the weight $W_{eq,2}(x,q)$).

The interest of $H_{x,2,n}(q/q_{eq})$ will be appreciated when treating the time evolution: see (36) below.

5. Time-dependent Wigner function W_2 up to order $\hbar^2$

5.1. Moments of W_2 using $H_{x,2,n}$ and three-term hierarchy

Let $W(x,q;t) \simeq W_2(x,q;t)$, where $W_2(x,q;t) \equiv W_2$ contains all contributions up to and including order $\hbar^2$, but disregards corrections of order $\hbar^{n''}$, $n'' \geq 3$. Accordingly, and based upon [19,20], by keeping up to and including order $\hbar^2$ but no more, we shall approximate Eq. (19) as:

$$\frac{\partial W_2}{\partial t} = -\frac{q}{m}\frac{\partial W_2}{\partial x} + \frac{dV}{dx}\frac{\partial W_2}{\partial q} - \frac{\hbar^2}{3!2^2}\frac{d^3V}{dx^3}\frac{\partial^3 W_2}{\partial q^3}. \tag{36}$$

If the $\hbar^2$ contribution (namely, $(\hbar^2/(3!2^2))(d^3V/dx^3)(\partial^3 W_2/\partial q^3)$) is neglected, Eq. (36) becomes the classical Liouville equation (2) with $W_2 = W_c$ (and $q = p$).

By using $H_{x,2,n}(q/q_{eq})$, we shall introduce the following moments $W_{2,n}$ ($n = 0, 1, 2, \ldots$) of the quantum Wigner function W_2 regarding the q-dependence:

$$W_{2,n} = W_{2,n}(x;t) = \int dq \frac{H_{x,2,n}(q/q_{eq})}{N_n(x)} W_2(x,q;t). \tag{37}$$

One has the following expansion for W_2:

$$W_2 = W_{eq,2}(x,q)\sum_{n=0}^{+\infty} W_{2,n}(x;t)\frac{H_{x,2,n}(q/q_{eq})}{N_n(x)}. \tag{38}$$

For $W_2 = W_{eq,2}(x,q)$, Eq. (37) yields $W_{eq,2,n} = 0$ if $n > 0$, and $W_{eq,2,0} = N_0(x)$ if $n = 0$.

Eq. (37), (36), (33) and (34) imply, through some lengthy algebra, the following infinite reversible three-term linear recurrence relation or hierarchy for all $N_nW_{2,n}$'s ($n = 0, 1, 2, \ldots, N_{-1}W_{2,-1} \equiv 0, a_2 = a_2(x), b_n = b_n(x)$):

$$\frac{\partial(N_nW_{2,n})}{\partial t} = -M_{n,n+1}N_{n+1}W_{2,n+1} - M_{n,n-1}N_{n-1}W_{2,n-1} \tag{39}$$

$$M_{n,n+1}N_{n+1}W_{2,n+1} \equiv \frac{q_{eq}}{2m}\frac{\partial(N_{n+1}W_{2,n+1})}{\partial x} \tag{40}$$

$$M_{n,n-1}N_{n-1}W_{2,n-1} \equiv \frac{q_{eq}n}{m}\frac{\partial((1+4a_2)N_{n-1}W_{2,n-1})}{\partial x} + \left[\frac{2n}{q_{eq}}\frac{\mathrm{d}V}{\mathrm{d}x} + \frac{q_{eq}}{2m}\frac{\mathrm{d}b_n}{\mathrm{d}x}\right]N_{n-1}W_{2,n-1}. \tag{41}$$

Undesirable contributions proportional to $W_{2,n-3}$ (with x-dependent coefficients) arise from $-(q/m)(\partial W_2/\partial x)$ and from the quantum correction $(\mathrm{d}^3V/\mathrm{d}x^3)(\partial^3W_2/\partial q^3)$. Fortunately, by using (23), (30) and (32), the two coefficients cancel out with each other, so that the overall contribution of $W_{2,n-3}$ vanishes exactly. This is a consequence of the use of the new moments (37) involving the $H_{x,2,n}$'s.

The initial quantum density operator is ρ_{in} at $t = 0$ which, through (18), yields W_{in}. The initial condition $N_nW_{in,2,n}$ for the recurrence (39) is obtained by replacing W_2 by W_{in} in (37) and retaining contributions up to order $\hbar^2$. In the classical limit, $a_2 = 0, b_n = 0$ $N_nW_{2,n} \to (\pi^{1/2}2^nn!)^{1/2}W_{c,n}$. One sees easily that Eq. (39) becomes Eq. (5).

The moments of $W_{eq,2}$, (that is, $W_{2,0} = W_{eq,2,0} = N_0(x)$ and $W_{2,n} = W_{eq,2,n} = 0$ for $n = 1, 2, \ldots$) yield a t-independent solution of Eq. (39).

5.2. Long-time approximations for three-term hierarchy

By extending the reduction of the Laplace transform of (5) to (10), the Laplace transform of (39) can also be transformed into another three-term hierarchy, which can be formally solved, by extending the procedures in Section 2, in terms of new infinite continued fractions of linear operators. The latter are more difficult to analyze than (13), due to the quantum corrections. Arguments aimed to give a more precise sense to the new infinite continued fractions are rather involved, and we shall omit them. It seems plausible that the classical arguments (leading to (14)) in Section 2 may, at least, give a useful hint when first quantum corrections are included (for adequately small β and $\hbar$).

In the simplest case, $n = 1$, we shall accept the approximate validity, for a long time, of:

$$N_1W_{2,1} \simeq -\frac{m}{\gamma_1}M_{1,0}N_0W_{2,0} \tag{42}$$

γ_1 being a real positive constant. (42) is some approximate counterpart, including first quantum corrections, of the inverse Laplace transform of (14), and its physical consistency will be confirmed below. By introducing (42) into (39) for $n = 0$, the resulting (irreversible) Smoluchowski equation for the distribution function $N_0W_{2,0}$ is:

$$\frac{\partial N_0W_{2,0}}{\partial t} = \frac{1}{\beta\gamma_1}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}((1+4a_2)N_0W_{2,0}) + \beta\frac{\mathrm{d}V}{\mathrm{d}x}N_0W_{2,0}\right] \tag{43}$$

with the initial condition $N_0W_{in,2,0}$ at $t = 0$. Thus, the long-time approximations in (42), without having assumed friction effects from the outset, have led to the Smoluchowski equation with first quantum corrections displayed in (43). An interesting check of consistency, a posteriori, is that (43) coincides with the Smoluchowski equation (also including first quantum corrections) obtained in [9] through a different procedure (involving ab initio friction effects). Again, the positive constant γ_1 in (43) plays the same role as the friction coefficient in [9]. $W_{2,0} = W_{eq,2,0}$ yields the t-independent solution of Eq. (43).

Next, let $n_0 = 2$, and approximate:

$$N_2W_{2,2} \simeq -\frac{m}{\gamma_2}M_{2,1}N_1W_{2,1} \tag{44}$$

γ_2 being a real positive constant. We replace (44) in Eq. (39) for $n = 1$. One finds:

$$\frac{\partial N_1W_{2,1}}{\partial t} = \frac{q_{eq}\gamma_2}{2}\frac{\partial}{\partial x}(M_{2,1}N_1W_{2,1}) - M_{1,0}N_0W_{2,0} \tag{45}$$

together with Eq. (39) for $n = 0$. Now, the initial condition is obtained from $W_{in,2,n}$, $n = 0, 1$, at $t = 0$. $W_{eq,2,0}$ and $W_{eq,2,1} = 0$ yield the t-independent solution of the set formed by (45) and (39) for $n = 0$.

The solutions of the above two simpler approximate closed hierarchies (namely, either (43) or (45) together with (39) for $n = 0$) relax irreversibly, for $t \gg 0$ and any reasonable $W_{in,2,n}$, towards the t-independent solutions, discussed above. This can be interpreted as the approximate irreversible evolution of the Brownian particle towards thermal equilibrium with the "heat bath" for long time, with first quantum corrections included.

6. Conclusions and discussions

New results have been reported for the dynamics of a quantum Brownian particle in a "heat bath" and an external potential, including the first quantum corrections. We have not assumed ab initio friction effects on the particle. Rather, we have extended methods previously reported for closed systems and for a classical Brownian particle [5,6], which yield approximate irreversible thermalization for a long time. For that purpose, using the equilibrium distribution as a weight function, we have introduced and analyzed a new family of orthogonal polynomials (the $H_{x,2,n}(q/q_{eq})$'s), which generalize the Hermite ones, and employed them to define new moments of the nonequilibrium distribution function. The standard Smoluchowski equations are recovered consistently for the lowest order moment, classically and quantum-mechanically. A possible applicability of the $H_{x,2,n}(q/q_{eq})$'s for quantum Brownian motion, when one includes a friction mechanism due to the "heat bath" from the outset, lies outside our scope here.

The following remarks (or, more properly, open questions) seem in order:

(a) The very fact that the $H_{x,2,n}(q/q_{eq})$'s fulfill the three-term recurrence relation (34) suggest that general techniques [25] could be applied to characterize the distributions of their zeroes. Such an analysis, as well as those of other properties of the $H_{x,2,n}(q/q_{eq})$'s, lie outside our scope here.

(b) The stationary states of the quantum-mechanical harmonic oscillator have information entropies, which are related to entropies involving the Hermite polynomials [26,27]. One could ask whether the Hermite polynomials and the above generalizations (including the first quantum corrections) and the associated moments are related to some information entropy in the actual Brownian motion framework.

From the contributions of orders $\hbar^2$ and $\hbar^4$ [19], it seems natural to infer that, to all orders in $\hbar^2$, $W_{eq}(x, q)$ can also be expressed as a series in Hermite polynomials H_{2n} of even order:

$$W_{eq}(x, q) = W_{c,eq} \sum_{n=0}^{+\infty} a_n(x) H_{2n}(q/q_{eq}). \tag{46}$$

In turn, the coefficients $a_n(x)$ are power series in $\hbar^2$, which depend on derivatives of $V(x)$ and on β. By generalizing what has been done in this work with the family of orthogonal polynomials $H_{x,2,n}(q/q_{eq})$ for $W_{eq,2}$, it could also be interesting to introduce the family of all orthogonal polynomials in q which have $W_{eq}(x, q)$, given by the infinite series (46) (including all orders in $\hbar^2$) as weight function, provided that one also integrates in $-\infty < q < +\infty$) and leaves x unintegrated. It is implicitly supposed that β and $\hbar$ are sufficiently small (and derivatives of V adequately smooth) for $W_{eq}(x, q)$ to be non-negative for any x and q. We denote those generalized polynomials as $H_{x,n}(q/q_{eq})$, $n = 0, 1, 2, 3, \ldots$. $H_{x,n}(q/q_{eq})$ depend parametrically on x, β and $\hbar$. Then, for $n \neq n'$ and any x:

$$\int \mathrm{d}q W_{eq}(x, q) H_{x,n}(q/q_{eq}) H_{x,n'}(q/q_{eq}) = 0. \tag{47}$$

By using the $H_{x,n}(q/q_{eq})$'s in order to define new moments (by generalizing (37)), Eq. (19) could be reduced to an exact linear recurrence relation for the new moments. All these also lie outside our scope here.

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