Semiclassical description of harmonic quantal Brownian motion

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By means of the Wigner transformation procedure, we extract a generalized Fokker-Planck equation that represents the semiclassical version of the quantal master equation for Brownian harmonic motion. The Fokker-Planck equation and its solutions are investigated both in the Markovian and in the non-Markovian regimes. The relations between semiclassical and classical Brownian motion of harmonic oscillators are analyzed with special emphasis on the high-friction limit.

I. INTRODUCTION

The theory of classical Brownian motion (CBM) was first investigated by Einstein¹ at the beginning of the century. From those early studies up to the present time, a lot of work has been published exploring the various features of CBM (see, for example, the review of Risken²). On the other hand, quantal motion in the presence of a heat bath, i.e., quantum Brownian motion (QBM) was first studied in the sixties,³⁻⁵ introducing the so-called quantum Langevin equation. Subsequently, many papers extending those early approaches were published, $^{6-9}$ dealing mainly with QBM of oscillators. Treatments of the damped harmonic oscillator have been also common in the context of quantum optics.¹⁰⁻¹⁴ In addition, the harmonic QBM can be regarded as an approach to the description of damped collective motion in finite quantal systems such as nuclei.¹⁵⁻¹⁸ In such a framework, the analysis of the relations between hydrodynamical and microscopic models is an interesting problem which may be explored through the extraction of semiclassical equations of motion from the quantum microscopic ones. Then, these semiclassical equations have to be analyzed focusing upon its classical or quasiclassical features in order to investigate a possible hydrodynamical description.19

In the present work, we have developed an investigation of the preceding type, specifically, we have explored the classical features of harmonic QBM. To this aim, we found it useful to consider an exact semiclassical version of the quantal equations which is obtained by means of the Wigner distribution function. $^{20-22}$ We prefer this quasiprobability representation to the Glauber-Sudarshan P function²³⁻²⁵ or other related representations,²⁶ which have been successfully applied to these kind of problems in quantum optics,^{11,12,26} since Wigner's distribution function has been shown to be a powerful tool in clarifying the connections between classical and quantum statistics.^{20,21} Actually, we show that Glauber's P function fulfills the same formal equation as Wigner's distribution. However, the former presents certain drawbacks related to its well-known²³ singularities appearing in the description of nonclassical states.²⁷ Particularly, it is remarkable that the P solutions for harmonic QBM at zero temperature are singular.²⁸

This paper is organized as follows. In Sec. II we extract, in the Markovian approximation, the semiclassical equation of motion which has, as expected,²¹ a Fokker-Planck structure. This equation is exactly solved and, in Sec. III we study the relation between the Markovian QBM and the high-friction CBM. In Sec. IV we consider the semiclassical version of the non-Markovian QBM finding the formal solution whose explicit form depends on the characteristics of the unspecified heat reservoir; however, an explicit solution which generalizes previous treatments^{29–31} can be obtained in a weak non-Markovian regime. In Sec. V we make a comparison between the non-Markovian QBM and the general CBM. Finally, the main results of this paper are discussed and summarized in Sec. VI.

II. SEMICLASSICAL VERSION OF THE QBM MASTER EQUATION

In this section we will consider the master equation that rules the motion of the phonon population $\rho_n(t)$, according to $^{10-12,28}$

$$\dot{\rho}_{n}(t) = W_{+}[(n+1)\rho_{n+1}(t) - n\rho_{n}(t)] + W_{-}[n\rho_{n-1}(t) - (n+1)\rho_{n}(t)], \qquad (2.1)$$

where W_{\pm} are constant transition rates whose detailed expression depends on the characteristics of the heat bath and its coupling to the oscillator. Equation (2.1) is the Markovian version of a more general non-Markovian one^{12,32,29-31} which will be considered in Sec. IV. The loss-of-memory-process undergone by an initial oscillator density $\rho_n(0)$ that moves according to (2.1) and the possibility of occurrence of non-Gibbsian equilibrium solutions have been discussed in Ref. 31.

Our current purpose is to derive the semiclassical counterpart of Eq. (2.1) according to Wigner.²⁰ Let us first consider the density operator $\hat{\rho} = \sum_{n=0}^{\infty} \rho_n |n\rangle \langle n|$, where $|n\rangle$ is a ket in the Fock basis. It is well known^{33,34} that the Wigner transform of the corresponding projector is

$$W(|n\rangle\langle n|) = (-1)^n 2L_n(4H/\hbar\Omega)\exp(-2H/\hbar\Omega) , \quad (2.2)$$

where $L_n(x)$ is the *n*th Laguerre polynomial and

<u>39</u> 2034

 $H = p^2/2m + (m/2)\Omega^2 q^2$ is the classical oscillator Hamiltonian. In turn, the *c* variables *p* and *q* are related to the Wigner transforms of the phonon creation and annihilation operators $\hat{\Gamma}^{\dagger}, \hat{\Gamma}$, since

$$W(\hat{\Gamma}) = \Gamma(q,p) = \left[\frac{m\Omega}{2\hbar}\right]^{1/2} q + \frac{ip}{\sqrt{2m\hbar\Omega}} . \qquad (2.3)$$

With this in mind, it is easy to compute the Wigner transform of the canonical distribution, actually the strongly stable fixed point of Eq. (2.1),

$$\hat{\rho}_0 = (1 - \beta) \sum_{n \ge 0} \beta^n |n\rangle \langle n| , \qquad (2.4)$$

with

$$\beta = W_{-} / W_{+} \quad . \tag{2.5}$$

Notice that the ratio β coincides with the Boltzmann factor $e^{-\hbar\Omega/kT}$, with T the equilibrium temperature of the heat bath, only if the coupling device is strictly energy-conserving;^{30,31} otherwise, the probabilistic parameter (2.5) depends on an extra microscopic energy coefficient related to the inelasticity width. In such a case one is entitled to speak of a non-Gibbsian behavior;^{5,30,31} however, this detail does not interfere with the foregoing analysis. Using expression (2.2) we find

$$\rho_0 = W(\hat{\rho}_0) = 2(1-\beta)e^{-2H/\hbar\Omega} \sum_{n \ge 0} (-\beta)^n L_n(4H/\hbar\Omega) .$$
(2.6)

Now the summation in (2.6) is just the generating function of the Laguerre polynomials,³⁵ provided that $\beta < 1$, a condition generally fulfilled on physical grounds.³¹ Consequently, we may write,

$$\rho_0(H) = 2 \frac{1-\beta}{1+\beta} \exp\left[-2 \frac{1-\beta}{1+\beta} \frac{H}{\hbar\Omega}\right].$$
 (2.7)

This result has been previously obtained^{36,21} using different methods. A look at Eq. (2.7) makes the following points apparent: (i) the semiclassical canonical distribution is isotropic in the (q,p) phase space; (ii) it is normalized, i.e., in angle-action variables,

$$\int \int \frac{dp \, dq}{h} \rho_0(H) = \int \int \frac{d\theta \, dH}{h\Omega} \rho_0(H) = 1 \quad ; \qquad (2.8)$$

(iii) the form (2.7) corresponds to a classical canonical distribution for an oscillator in equilibrium at an effective temperature $T_{\rm eff}$ given by

$$kT_{\rm eff} = \frac{\hbar\Omega}{2} \frac{1+\beta}{1-\beta} = \frac{\hbar\Omega}{2} \frac{W_+ + W_-}{W_+ - W_-} . \tag{2.9}$$

The actual temperature T of the heat reservoir, as well as the typical energy parameters of the coupling mechanism, enter the structure of this effective temperature through the microscopic transition probabilities W_{\pm} . In particular realizations of these rates, one could analyze whether the actual temperature T coincides or not with the effective temperature, namely, with the equilibrium parameter of the semiclassical counterpart of the quantal canonical density regarded as canonical in classical phase space. One may visualize expression (2.9) as preserving, through the "Wignerization" procedure, the basic quantal nature of the system.

We are now ready to analyze the Wigner transform of Eq. (2.1). If we take into account that (2.1) is the diagonal matrix element of the operator equation 10-12,28

$$\hat{\rho} = \frac{1}{2} W_{+} (2\hat{\Gamma}\hat{\rho}\hat{\Gamma}^{\dagger} - \hat{\rho}\hat{\Gamma}^{\dagger}\hat{\Gamma} - \hat{\Gamma}^{\dagger}\hat{\Gamma}\hat{\rho}) + \frac{1}{2} W_{-} (2\hat{\Gamma}^{\dagger}\hat{\rho}\hat{\Gamma} - \hat{\Gamma}\hat{\Gamma}^{\dagger}\hat{\rho} - \hat{\rho}\hat{\Gamma}\hat{\Gamma}^{\dagger})$$
(2.10)

and examine the form of the Wigner transform of any threefold product in (2.10), employing standard product rules, ^{33,36,37} we readily conclude that an expansion up to order \hbar^2 yields the exact result for the required transform. This is a consequence of the fact that the semiclassical phonon operator $\Gamma(q,p)$ in Eq. (2.3) possesses vanishing second derivatives in phase space. After some algebra, the final result is easily expressed in action variable representation as

$$\frac{\partial \rho}{\partial t} = v \left[\rho + (H + kT_{\text{eff}}) \frac{\partial \rho}{\partial H} + kT_{\text{eff}} H \frac{\partial^2 \rho}{\partial H^2} \right], \quad (2.11)$$

where

$$v = W_{+} - W_{-}$$
 (2.12)

and with kT_{eff} given in Eq. (2.9). We note that the missing angle in Eq. (2.11) is thoroughly related to the missing off-diagonal matrix elements in Eq. (2.1).

An equation of similar form rules the motion of the Glauber-Sudarshan²³⁻²⁵ quasiprobability distribution function $P(\alpha)$. In fact, this equation can be obtained from (2.11) by means of the formal replacements²⁸

$$\rho \rightarrow P$$
, (2.13a)

$$H \rightarrow |\alpha|^2$$
, (2.13b)

$$kT_{\rm eff} \rightarrow n_{\rm TH} = (\beta^{-1} - 1)^{-1}$$
 (2.13c)

The correspondence (2.13b) is not surprising if we recall that the complex variable α is associated to the coherent state $|\alpha\rangle$ which fulfills

$$\langle \alpha | \hat{H}_{\text{osc}} | \alpha \rangle \sim | \alpha |^2$$
 (2.14)

in the classical limit $|\alpha|^2 >> 1$.

Notice in (2.13c) that kT_{eff} must be replaced by the number of thermal phonons which vanishes for $\beta \rightarrow 0$, i.e., for a configuration of vanishing equilibrium temperature. On the other hand, kT_{eff} [Eq. (2.9)] tends in that case to the zero-point energy $\hbar\Omega/2$. This different behavior of both parameters have important consequences as will be shown in what follows. In fact, (2.11) has the form of a one-dimensional Fokker-Planck equation (FPE) with variable drift and diffusion coefficients.² One can straightforwardly verify that it can be written in the standard manner,

$$\frac{\partial \rho(H,t)}{\partial t} = -\frac{\partial}{\partial H} [D^{(1)}(H)\rho(H,t)] + \frac{\partial^2}{\partial H^2} [D^{(2)}(H)\rho(H,t)], \qquad (2.15)$$

with the rates

$$D^{(1)}(H) = v(kT_{\text{eff}} - H)$$
, (2.16a)

$$D^{(2)}(H) = vkT_{eff}H$$
 (2.16b)

Then, in Glauber's picture, the diffusion coefficient (2.16b) becomes proportional to the number of thermal phonons (2.13c) which may vanish leading to a singular diffusionless FPE. On the other hand, the diffusion coefficient in Wigner's representation remains definite positive for any temperature. We may conclude that this behavior is showing the well-known drawbacks of the P function for describing nonclassical configurations.^{23,26,21,31} The general solution of (2.11) can be spectrally decomposed as

$$\rho(H,t) = \sum_{l \ge 0} A_l e^{-l_V t} e^{-H/kT_{\text{eff}}} L_l(H/kT_{\text{eff}}) , \qquad (2.17)$$

with the amplitudes related to the initial condition $\rho(H,0)$ in the usual way,

$$A_{l} = \int_{0}^{\infty} dx \ L_{l}(x) \rho(kT_{\text{eff}}x, 0) \ . \tag{2.18}$$

The validity of decomposition³⁸ (2.17) is asserted in Appendix A. Since $L_0(x) = 1$, we have

$$\frac{kT_{\text{eff}}}{\hbar\Omega} A_0 = \frac{kT_{\text{eff}}}{\hbar\Omega} \int_0^\infty dx \,\rho(kT_{\text{eff}}x,0) = W[\operatorname{Tr}\hat{\rho}(0)] = 1 \,.$$
(2.19)

This normalization condition persists during the evolution; indeed, (2.17) allows us to write

$$\int_{0}^{\infty} dx \,\rho(kT_{\text{eff}}x,t) = \sum_{l \ge 0} A_{l}e^{-l\nu t} \int_{0}^{\infty} dx \,e^{-x}L_{l}(x)L_{0}(x)$$
$$= \sum_{l \ge 0} A_{l}e^{-l\nu t}\delta_{l_{0}} = A_{0} \,. \tag{2.20}$$

It is also important to notice that, as expected, the spectrum of eigenvalues of the semiclassical QBM is identical to the spectrum of the Markovian master equation,³¹ being both of them,³⁹

$$\lambda_l = -l\nu = -l(W_+ - W_-); \quad l = 0, 1, 2, \dots$$
 (2.21)

III. RELATION OF THE SEMICLASSICAL QBM TO THE HIGH-FRICTION CBM

The general one-dimensional FPE (2.15), with drift and diffusion rates given in (2.16), admits a further transformation. Indeed, the semiclassical Brownian motion described by this equation is related to a classical, constant-diffusion process undergone by a variable y(H) defined as²

$$y(H) = \int_0^H dz [D/D^{(2)}(z)]^{1/2}, \qquad (3.1)$$

with D an arbitrary positive scaling constant, i.e.,

$$H = \frac{vkT_{\text{eff}}y^2}{4D} . \tag{3.2}$$

One can then extract, out of (2.11) or (2.15), the equation

$$\frac{\partial \rho}{\partial t}(y,t) = v\rho(y,t) + \left[\frac{D}{y} + \frac{vy}{2}\right] \frac{\partial \rho(y,t)}{\partial y} + D \frac{\partial^2 \rho(y,t)}{\partial y^2} .$$
(3.3)

A FPE is not immediately recognized in (3.3); however, one more transformation to a deformed distribution

$$R(y,t) = \frac{\nu k T_{\text{eff}}}{2D} y \rho(y,t)$$
(3.4)

permits us to write Eq. (3.3) in the form

$$\frac{\partial R(y,t)}{\partial t} = -\frac{\partial}{\partial y} [d^{(1)}(y)R(y,t)] + D \frac{\partial^2 R(y,t)}{\partial y^2} , \qquad (3.5)$$

with the new drift parameter

$$d^{(1)}(y) = \frac{D}{y} - \frac{v}{2}y \quad . \tag{3.6}$$

It is interesting to notice that, since this coefficient vanishes for $y^2 = 2D/\nu$, corresponding to $H = kT_{\text{eff}}/2$, the FPE (3.5) is locally a pure diffusion equation with a constant diffusion rate D.

Expression (3.5) is a Smoluchowski equation that describes the classical Brownian motion (CBM) of a onedimensional oscillator in the high-friction limit.² The variable y is the oscillator coordinate, in such a case, and the drift parameter (3.6) is proportional to the ratio of a conservative force to a dissipative one with friction strength η

$$d^{(1)}(y) = F(y) / M \eta$$
, (3.7)

where M is the oscillator mass. The conservative force may be derived from the potential

$$V(y) = -\int_0^y F(z)dz = (M\eta v/4)y^2 - M\eta D \ln y . \qquad (3.8)$$

We can then appreciate that, in view of the origin of Eq. (3.5), which arises, after a series of transformations, from the semiclassical counterpart of the QBM master equation, we are left with a family of classical oscillators of frequency $w = (\eta v/2)^{1/2}$ and mass M (the parameters of the family being η and M) placed in the field of a linear source with strength $MD\eta$. This strength is arbitrary, however nonvanishing; its actual value is unimportant, as one realizes after examination of the equilibrium solution of (3.5). This solution corresponds to zero current S(y), with

$$S(y) = D \frac{\partial R(y)}{\partial y} - d^{(1)}(y)R(y) . \qquad (3.9)$$

For vanishing S(y), one finds,

$$R_0(y) \sim \exp\left[\int_0^y \frac{d^{(1)}(z)}{D} dz\right] = \exp\left[-V(y)/M\eta D\right],$$
(3.10)

from where we obtain

$$R_0(y) \sim y \exp\left[-\frac{vy^2}{4D}\right]$$
. (3.11)

SEMICLASSICAL DESCRIPTION OF HARMONIC QUANTAL ...

After normalization of (3.11), using (3.2) and (3.4) we recover the classical equilibrium distribution (2.7),

$$\rho_0(H) = \frac{\hbar\Omega}{kT_{\rm eff}} \exp(-H/kT_{\rm eff}) . \qquad (3.12)$$

From the preceding discussion, we see that the value of the constant D itself is unimportant, since it plays the role of a scaling factor in a change of variables when going from the FPE (2.15) to the Smoluchowski one (3.5). However, if we recall that in the description of CBM of an oscillator, the fluctuation-dissipation theorem relates the diffusion parameter to the friction coefficient. by means of the equilibrium temperature as

$$D = kT_{\rm eff} / M\eta , \qquad (3.13)$$

it becomes apparent from the expression of the effective conservative potential (3.8) that the logarithmic deformation with respect to the harmonic potential occurs with intensity kT_{eff} . In fact, this singularity arises from the Jacobian of the nonlinear change of variables (3.2); we further recognize that, if we adopt the fluctuationdissipation rule (3.13), the preceding change of variables reads,

$$H = M \eta \frac{\nu}{4} y^2 . \qquad (3.14)$$

The latter expression and (3.8) show once again that the variable y is the position coordinate of an oscillator with mass M and frequency $\omega = (\eta v/2)^{1/2}$ that performs CBM while stimulated by a logarithmic singularity $-kT_{\text{eff}} \ln y$. Indeed, in the high-friction limit, the kinetic energy of an oscillator adds a negligible contribution to the potential energy (3.14).

Let us now briefly consider the spectrum of the Smoluchowski equation for a free harmonic oscillator, i.e., with a drift coefficient [cf. (3.6)]

$$d_0^{(1)}(y) = -\frac{\nu}{2}y = -\frac{\omega^2}{\eta}y \quad . \tag{3.15}$$

This equation is

$$\frac{\partial \rho}{\partial t}(y,t) = \frac{\omega^2}{\eta} \rho(y,t) + \frac{\omega^2}{\eta} y \frac{\partial \rho}{\partial y}(y,t) + \frac{kT_{\text{eff}}}{M\eta} \frac{\partial^2 \rho(y,t)}{\partial y^2}$$
(3.16)

and is identical to the FPE in velocity space for a particle of mass $M(\eta/\omega)^2$ undergoing CBM with a friction parameter $\eta' = \omega^2/\eta$ (cf. Ref. 2). It is straightforward to find stationary solutions of (3.16) of the form

$$\rho_{l}(y,t) = \exp\left[-l\frac{\omega^{2}}{\eta}t - \frac{M\omega^{2}y^{2}}{2kT_{\text{eff}}}\right]H_{l}\left[\left[\frac{M\omega^{2}}{2kT_{\text{eff}}}\right]^{1/2}y\right],$$
(3.17)

with $H_l(x)$ the *l*th Hermite polynomial.³⁵

We realize that the eigenvalues $K_l = -l\omega^2/\eta$ are just one half of the eigenvalues λ_l [cf. Eqs. (2.21) and (3.15)] of the Smoluchowski equation (3.5), since the latter is equivalent to the FPE that represents the semiclassical version of the QBM. This difference should thus be ascribed to the logarithmic singularity, that is missing in the CBM problem (3.16). One could then speculate that such a singularity is deeply connected to the basic quantal nature of the system undergoing the semiclassical motion (3.5).

IV. SEMICLASSICAL VERSION OF THE NON-MARKOVIAN QBM MASTER EQUATION

The generalization of the master equation (2.1) to non-Markovian situations^{12,32,29–31} leads to the integrodifferential operator equation [cf. Eq. (2.10)]

$$\dot{\hat{\rho}}(t) = \int_{0}^{t} d\tau \{ \frac{1}{2} W_{+}(\tau) [2\hat{\Gamma}\hat{\rho}(t-\tau)\hat{\Gamma}^{\dagger} - \hat{\rho}(t-\tau)\hat{\Gamma}^{\dagger}\hat{\Gamma} - \hat{\Gamma}^{\dagger}\hat{\Gamma}\hat{\rho}(t-\tau)] + \frac{1}{2} W_{-}(\tau) [2\hat{\Gamma}^{\dagger}\hat{\rho}(t-\tau)\hat{\Gamma} - \hat{\Gamma}\hat{\Gamma}^{\dagger}\hat{\rho}(t-\tau) - \hat{\rho}(t-\tau)\hat{\Gamma}\hat{\Gamma}^{\dagger}] \}, \qquad (4.1)$$

where $W_{\pm}(\tau)$ are the instantaneous transition rates, similar to the constant ones in Eq. (2.1), whose explicit form depends on the characteristics of the heat bath and its coupling to the oscillator. The Wigner transform of Eq. (4.1) is easily obtained by the same method which led from Eq. (2.10) to Eq. (2.11) yielding a non-Markovian FPE,

$$\frac{\partial \rho(H,t)}{\partial t} = \int_0^t d\tau \left[(W_+ - W_-)_\tau \rho(H,t-\tau) + \left[(W_+ - W_-)_\tau H + \frac{\hbar\Omega}{2} (W_+ + W_-)_\tau \right] \frac{\partial \rho(H,t-\tau)}{\partial H} + \frac{\hbar\Omega}{2} H (W_+ + W_-)_\tau \frac{\partial^2 \rho(H,t-\tau)}{\partial H^2} \right].$$
(4.2)

Taking into account the convolution form of the right-hand side of Eq. (4.2) it is convenient, in order to solve this equation, to perform a Laplace transformation, introducing the complex density

$$\rho(H,\lambda) = \int_0^\infty d\tau e^{-\lambda\tau} \rho(H,\tau)$$
(4.3)

The transformed equation from (4.2) reads

2037

2038

E. S. HERNÁNDEZ AND H. M. CATALDO

where W_{\pm} are here the Laplace transforms of the timedependent $W_{\pm}(\tau)$ and represent transition ratelike functions $W_{\pm}(\lambda)$. Equation (4.4) for the transformed density $\rho(H,\lambda)$ can be written as follows:

$$kT_{\rm eff}H\frac{\partial^2\rho(H,\lambda)}{\partial H^2} + (H + kT_{\rm eff})\frac{\partial\rho(H,\lambda)}{\partial H} + \left(1 - \frac{\lambda}{W_+ - W_-}\right)\rho(H,\lambda) + \frac{\rho(H,t=0)}{W_+ - W_-} = 0,$$
(4.5)

where kT_{eff} now represents a complex temperaturelike function [cf. Eq. (2.9)]

$$kT_{\rm eff} \equiv kT_{\rm eff}(\lambda) = \frac{\hbar\Omega}{2} \frac{W_+(\lambda) + W_-(\lambda)}{W_+(\lambda) - W_-(\lambda)} . \qquad (4.6)$$

In Appendix B we show that the general solution of Eq. (4.5) can be obtained under the restriction

$$\operatorname{Re}[kT_{\text{eff}}(\lambda)] > 0 ; \qquad (4.7)$$

this solution reads

$$\rho(H,\lambda) = \exp(-H/kT_{\text{eff}})$$

$$\times \sum_{n \ge 0} \frac{1}{(W_{+} - W_{-})n + \lambda} A_{n}(\lambda) L_{n}(H/kT_{\text{eff}}) ,$$
(4.8)

with the amplitudes $A_n(\lambda)$ related to the initial condition $\rho(H, t=0)$,

$$A_n(\lambda) = \frac{1}{kT_{\text{eff}}} \int_0^\infty \rho(H, t=0) L_n(H/kT_{\text{eff}}) dH \quad . \tag{4.9}$$

Taking into account Eqs. (4.7), (4.8), and (4.9) we realize that the only poles of $\rho(H,\lambda)$ are the roots of the equation [cf. Eq. (2.21)]

$$\lambda = n \left[W_{-}(\lambda) - W_{+}(\lambda) \right] \tag{4.10}$$

for n = 0, 1, 2, ... Finally, antitransformation of Eq. (4.8) yields the desired expression for the time evolution

$$\rho(H,t) = \sum_{n_i \ge 0} e^{\lambda_{n_i} t} \operatorname{Res} \left[\frac{1}{\lambda - n \left(W_- - W_+ \right)}, \lambda_{n_i} \right]$$
$$\times \exp[-H/k T_{\text{eff}}(\lambda_{n_i})]$$
$$\times L_n [H/k T_{\text{eff}}(\lambda_{n_i})] A_n(\lambda_{n_i}), \quad (4.11)$$

where λ_{n_i} denotes the *i*th root of Eq. (4.10).⁴⁰ From expression- (4.11) we may realize that the property (4.7) preserves the boundary condition of the Wigner distribution function⁴¹

$$\lim_{H \to \infty} \rho(H,t) = 0 . \tag{4.12}$$

Actually, from Eq. (4.6) it is easy to see that (4.7) is equivalent to the condition

$$|\boldsymbol{\beta}(\boldsymbol{\lambda})|^2 < 1 , \qquad (4.13)$$

where

$$\beta(\lambda) \equiv W_{-}(\lambda) / W_{+}(\lambda) . \qquad (4.14)$$

In Ref. 31 it has been shown that condition (4.13) ensures the convergence of the solutions of the non-Markovian QBM master equation.

The equation (4.10) which gives the non-Markovian frequencies has been specially studied considering a fermionic reservoir whose particles interact with the phonons of the oscillator through inelastic collisions.²⁹⁻³¹ In this case, the functions $W_+(\lambda)$ take the explicit form

$$W_{\pm}(\lambda) = 2g^2 / \hbar^2 \sum_{\alpha\mu} |\lambda_{\alpha\mu}|^2 \frac{(\gamma + \lambda)}{(\gamma + \lambda)^2 + (\omega_{\alpha\mu} - \Omega)^2} \times \begin{cases} \rho_{\mu}(1 - \rho_{\alpha}) \\ \rho_{\alpha}(1 - \rho_{\mu}) \end{cases}, \qquad (4.15)$$

where g is a spin-isospin degeneracy factor, γ is the inelasticity width whose inverse $\gamma^{-1} = \tau_{corr}$ represents a correlation time or lifetime of a microscopic particlephonon collision, $\omega_{\alpha\mu} = (\epsilon_{\alpha} - \epsilon_{\mu})/\hbar$ with ϵ_A a singleparticle energy, ρ_A is a Fermi equilibrium distribution at a temperature T as a function of ϵ_A , and $\lambda_{\alpha\mu}$ are interaction matrix elements.

In Eq. (4.15) we can recognize a generic structure which does not depend on the fermionic nature of the heat bath,

$$W(\lambda) = \sum_{P} \frac{(\gamma + \lambda)}{(\gamma + \lambda)^2 + (\Delta \varepsilon_P / \hbar)^2} W_P , \qquad (4.15')$$

where the summation involves only phonon creation (annihilation) processes for W_- (W_+). The energy difference $\Delta \varepsilon_P$ measures the inelasticity of the process p, which has, as well as all of them, a characteristic inelasticity width given by the parameter $\hbar \gamma$. Each process p is weighted in Eq. (4.15') by a coefficient W_p which generally depends on the density matrix of the heat bath and on the interaction Hamiltonian.

The inelasticity parameter $\hbar\gamma$ accounts for energy losses in general. For instance, inelasticity could arise from unspecified heat baths which are coupled to the system. In this case, γ^{-1} should represent the fastest dissipative relaxation time introduced by these reservoirs.^{42,43} Another physical realization of the inelasticity involves certain hidden degrees of freedom or unobserved interaction channels which, however, are participating in the

<u>39</u>

overall relaxation process.^{29-31,19}

Now we will focus upon the most common situation where one has a phonon frequency Ω much smaller than the inelasticity width γ , however, we must point out that this assumption does not lead to the Markovian limit.³⁰ In fact, one may realize that expression (4.15') can be approximated by

$$W(\lambda) \approx \frac{1}{\gamma + \lambda} \sum_{P} W_{P}$$
 (4.16)

since

$$\Omega^2 \sim (\Delta \varepsilon_P / \hbar)^2 \ll |\gamma + \lambda|^2 . \tag{4.17}$$

The validity of Eq. (4.16) for λ not very close to $-\gamma$ has been tested in Ref. 30. Assumption (4.16) causes Eq. (4.14) to become independent of λ and equal to the generalized Boltzmann factor (2.5). Therefore if the total weight $(\sum_{P} W_{P})$ of phonon-annihilation processes is larger than the corresponding quantity for phononcreation processes (this condition could establish certain selection rules on the interaction matrix elements³¹), then condition (4.13) is fulfilled. Equation (4.10) can be written, using (4.16), as

$$\lambda \approx \frac{n}{\gamma + \lambda} (A_{-} - A_{+}) = \frac{-nA}{\gamma + \lambda} , \qquad (4.18)$$

where we have $A_{+} - A_{-} = A > 0$ according to (4.13). The roots of (4.18) can be easily obtained giving

$$\lambda_n^{\pm} = -\gamma / 2 \pm \left[\frac{\gamma^2}{4} - nA \right]^{1/2}$$
 (4.19)

The Markovian limit arises from Eq. (4.19) in the overdamped case with high inelasticity,^{29,30} i.e., $4n A / \gamma^2 \ll 1$, then we must neglect one of the roots, namely, that near $-\gamma$ and the other one yields the Markovian spectrum [cf. Eq. (2.21)]

$$\lambda_n^+ \simeq -n A / \gamma \quad . \tag{4.20}$$

Now, taking into account the approximation (4.16)-(4.19) it is easy to calculate the residues in Eq. (4.11),

$$\operatorname{Res}(\lambda_n^{\pm}) = \frac{\alpha_n \pm 1}{2\alpha_n} , \qquad (4.21)$$

where

$$\alpha_n = (1 - 4n A / \gamma^2)^{1/2} . \tag{4.22}$$

We can see from (4.21) that, in the Markovian limit $(4n A / \gamma^2 \ll 1)$, the residue of the Markovian pole (4.20) tends to unity while the residue of the spurious pole λ_n^- is negligible. Finally, using the preceding results, we can get an explicit expression for (4.11),

$$\rho(H,t) = \sum_{n \ge 0} A_n e^{-(\gamma/2)t} \left[\cosh\left[\frac{\gamma}{2}\alpha_n t\right] + \frac{1}{\alpha_n} \sinh\left[\frac{\gamma}{2}\alpha_n t\right] \right]$$
$$\times e^{-H/kT_{\text{eff}}} L_n(H/kT_{\text{eff}}), \qquad (4.23)$$

where one may verify that the reality of the Wigner distribution function²⁰ is preserved, since, according to (4.22), the coefficients α_n can only assume real or imaginary values. We must remark that the result (4.23), which generalizes the Markovian one given in Eq. (2.17), was derived under the hypothesis (4.17) ($\Omega \ll \gamma$) and is therefore valid in a weak non-Markovian regime.

A non-Markovian approach to harmonic QBM was investigated earlier by Haake.³² In that work, he considered a harmonic oscillator coupled to a bath of harmonic oscillators and, since this problem is exactly solvable, he could test the validity of the Born approximation.⁴⁴ He extracted (in a weak non-Markovian regime) analytical expressions for the relaxation frequencies corresponding to the energy (mean number of phonons) which, in our approach, correspond to n = 1 in Eq. (4.19).^{29,31} It is not possible to perform an explicit comparison between these results and those of the present paper, since the non-Markovian analysis is strongly dependent on the assumptions regarding the reservoirs and the interactions. However, it is worthwhile noticing that in both works one finds that the non-Markovian regime presents damped oscillations which otherwise remain unobserved in the Markovian approximation (see Sec. V).

V. RELATION OF THE SEMICLASSICAL NON-MARKOVIAN QBM TO THE GENERAL CBM

The motion of a classical harmonic oscillator in a heat bath subjected to friction-plus-Gaussian random forces is described by the Kramers equation²

$$\frac{\partial \rho(x,v,t)}{\partial t} = -\frac{\partial}{\partial x}v\rho + \frac{\partial}{\partial v}(\eta v + \omega^2 x)\rho + \eta \frac{kT}{M} \frac{\partial^2 \rho}{\partial v^2} .$$
(5.1)

Here $\rho(x,v,t)$ is the probability density in phase space (x,p/M). The spectral problem of this equation is also known and we recall the eigenvalues²

$$\lambda_{n_1 n_2} = -\frac{1}{2} \eta (n_1 + n_2) - \frac{1}{2} (\eta^2 - 4\omega^2)^{1/2} (n_1 - n_2)$$
(5.2)

for non-negative integers n_1 and n_2 . We may recognize the high-friction limit $4\omega^2/\eta^2 \ll 1$, namely, a special limit of the overdamped case,

$$\lambda_{n_1 n_2}^{\rm HF} \approx -\eta n_1 (1 - \omega^2 / \eta^2) - n_2 \omega^2 / \eta$$
, (5.3)

and observe that the spectrum of the Smoluchowski equation (3.16) is precisely the highest-lying branch (lowest absolute value of the eigenvalues), $n_1 = 0$. We recall the existing isomorphism between the latter spectrum and that of the Markovian QBM which was discussed at length in Sec. III. Although in the high-friction CBM as well as in the Markovian QBM two very different time scales arise, we must remark that Kramers equation for general CBM does not involve any non-Markovian hypothesis.⁴⁵ In fact, it arises from a Langevin equation driven by Gaussian white noise and it is well known⁴⁶ that such processes imply Markovianity.

We find also similarities between the spectra (4.19) and (5.2); they possess damping parameters, namely, $4 A / \gamma^2$ and $4\omega^2/\eta^2$, respectively, which if larger than unity lead to an underdamped regime, i.e., only complex frequencies. However, we must point out the different structure of both damping parameters; in the classical case, $4\omega^2/\eta^2$ is proportional to the square of the oscillator frequency, on the other hand, in the QBM, A is proportional to the square of the interaction matrix elements [cf. Eqs. (4.15) and (4.15')]. Another difference between CBM and QBM arises from the fact that the latter does not possess a properly overdamped regime, since Eq. (4.19) always can give complex frequencies for large enough n.

VI. SUMMARY

We have extracted the semiclassical (Wigner) description of the QBM master equation in both the Markovian approximation and the full non-Markovian version. In the Markovian regime, the equation of motion for the Wigner distribution function of the quantal oscillator is a general FPE with variable diffusion and drift parameters, whose spectrum of eigenvalues coincides with that of the QBM master equation and whose equilibrium solution is the Wigner transform of the quantal equilibrium density operator. The semiclassical equilibrium distribution is the canonical one for an oscillator in phase space, however, the temperature parameter is different from the actual temperature of the heat bath. More specifically, the effective equilibrium temperature $T_{\rm eff}$ of the oscillator in phase space contains the microscopic transition rates that govern the original master equation.

Furthermore, one can find, after some simple analytical transformations, that the preceding FPE can be carried into the form of a Smoluchowski equation describing the CBM of an oscillation in the high-friction limit. One realizes that there exists a family of classical oscillators, parameterized by the mass and friction strengths, to which the given Smoluchowski equation applies. Each member of this family could be regarded as a semiclassical image of the original quantal system; however, the position coordinate of the image is nonlinearly related to the energy of the source oscillator, rather than to its coordinate. As a consequence of such a change of variables, an extra singular potential appears where the image is placed, namely, a logarithmic singularity. It is shown that the effect of this singularity is to double the eigenvalues of this Smoluchowski equation with respect to those of the free harmonic oscillator, a fact that can be regarded as a signal of the underlying quantal nature of the system.

The full non-Markovian QBM master equation transforms, under the same procedure, in a non-Markovian general FPE which, after a Laplace transformation, adopts the same form of the eigenvalue equation related to the Markovian FPE. The only difference resides in the fact that this eigenvaluelike equation is nonlinear, its roots being the resolvent poles. When the non-Markovianity is weak, i.e., when the macroscopic period exceeds the typical correlation time (however not to an extent sufficient to consider a Markovian limit) the resolvent poles can be analytically written down. One then realizes that the non-Markovian spectrum of decay rates shows different damping regimes, in close analogy to the classical spectrum of the Kramers equation.

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APPENDIX A: SOLUTION OF THE SPECTRAL PROBLEM OF THE MARKOVIAN FOKKER-PLANCK EQUATION

In this appendix we compute the eigenfunctions of the FPE (2.11). Changing variables to $x = H/kT_{\text{eff}}$, the latter reads

$$\frac{\partial \rho(x, vt)}{\partial (vt)} = \rho + (1+x)\frac{\partial \rho}{\partial x} + x\frac{\partial^2 \rho}{\partial x^2} .$$
 (A1)

Looking now for stationary solutions of the form $\rho(x, \nu t) = \exp(-\lambda \nu t)\rho_{\lambda}(x)$, one finds the secular equation

$$x\rho_{\lambda}^{\prime\prime} + (1+x)\rho_{\lambda}^{\prime} + (1+\lambda)\rho_{\lambda} = 0$$
 (A2)

Under the substitution $\rho_{\lambda}(x) = e^{-x} r_{\lambda}(x)$, one arrives to the Laguerre equation for non-negative integer $\lambda = l_{\lambda}^{35}$

$$xr_l'' + (1-x)r_l' + lr_l = 0 , \qquad (A3)$$

with solutions $r_l(x) = L_l(x)$ (the *l*th Laguerre polynomial). Consequently, the eigenfunctions of the FPE (A1) are

$$\rho_l(\mathbf{x}) = e^{-\mathbf{x}} L_l(\mathbf{x}) \tag{A4}$$

and any initial distribution $\rho(x,0)$ that admits an expansion in terms of these eigenfunctions evolves in time, according to (A1), as stated by the superposition principle,

$$\rho(x,t) = \sum_{l \ge 0} e^{-l\nu t} e^{-x} L_l(x) \int_0^\infty dy \, \rho(y,0) L_l(y) \,. \quad (A5)$$

APPENDIX B: SOLUTION OF THE EQUATION FOR THE LAPLACE-TRANSFORMED DENSITY

In this appendix we will show the steps leading to the general solution of Eq. (4.5). First we propose the substitution

$$\rho(H,\lambda) = e^{-H/kT_{\rm eff}(\lambda)} R(H,\lambda) , \qquad (B1)$$

which transforms Eq. (4.5) into

SEMICLASSICAL DESCRIPTION OF HARMONIC QUANTAL ...

$$0 = \frac{\exp(H/kT_{\text{eff}})\rho(H, t=0)}{W_{+} - W_{-}} - \frac{\lambda R(H,\lambda)}{W_{+} - W_{-}} + (kT_{\text{eff}} - H)\frac{\partial R}{\partial H} + kT_{\text{eff}}H\frac{\partial^{2}R}{\partial H^{2}}.$$
 (B2)

Now, if we use the ansatz

$$R(H,\lambda) = \sum_{n \ge 0} C_n L_n (H/kT_{\text{eff}}) , \qquad (B3)$$

where $L_n(x)$ is the *n*th Laguerre polynomial, the Eq. (B2) yields

$$\exp(H/kT_{\text{eff}})\frac{\rho(H, t=0)}{W_{+}-W_{-}} = \sum_{n \ge 0} \left[n + \frac{\lambda}{W_{+}-W_{-}} \right] C_{n}$$
$$\times L_{n}(H/kT_{\text{eff}}) . \tag{B4}$$

Now, the orthogonality relation

$$\frac{1}{kT_{\text{eff}}} \int_0^\infty \exp(-H/kT_{\text{eff}}) L_j (H/kT_{\text{eff}}) L_n (H/kT_{\text{eff}}) dH$$
$$= \delta_{jn} \qquad (B5)$$

holds if and only if

$$\operatorname{Re}[kT_{\text{eff}}(\lambda)] > 0 . \tag{B6}$$

Hence, the assumption (B6) allows us to extract the coefficients C_n of the ansatz (B3) from Eq. (B4) as

$$C_{n} = [(W_{+} - W_{-})n + \lambda]^{-1} (kT_{\text{eff}})^{-1} \\ \times \int_{0}^{\infty} \rho(H, t = 0) L_{n} (H/kT_{\text{eff}}) dH , \qquad (B7)$$

which leads to the general solution (4.8).

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