# Application of the generalized Feynman-Vernon approach to a simple system: The damped harmonic oscillator

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We apply a recently developed generalization of the Feynman-Vernon approach to the case of a quantum-mechanical damped oscillator. We develop a variational method to treat the path integral that controls the dynamics of the reduced density operator of the system once it is subject to an arbitrary initial condition. The method is completely independent of the specific symmetries involved in the problem. Although we have applied it particularly to the harmonic oscillator, we believe it could be extended to more complex systems.

#### I. INTRODUCTION

During the past five years the Feynman-Vernon approach to the quantum dynamics of nonisolated systems<sup>1,2</sup> has proved to be a very powerful method in this field. It can be applied to many different problems such as quantum dynamics of a dissipative system in the classically accessible region of the phase space,<sup>3</sup> quantum tunneling of a dissipative system (dynamical approach),<sup>4</sup> damping of quantum interference,<sup>5</sup> or damping of quantum coherence.<sup>6</sup>

The method consists of coupling the system of interest to a reservoir which is conveniently chosen as a set of Nnoninteracting oscillators. The coupling between the two systems is a bilinear function of the "coordinates" of the system of interest and the reservoir oscillators. If the system of interest is represented by a particle of coordinate q, the Lagrangian of the total system is

$$L = \frac{1}{2}m\dot{q}^{2} - V(q) + \sum_{k} C_{k}q_{k}q + \sum_{k} \frac{1}{2}m_{k}\dot{q}_{k}^{2} - \sum_{k} \frac{1}{2}m_{k}\omega_{k}^{2}q_{k}^{2}$$
$$- \frac{1}{2}\sum_{k} \frac{C_{k}^{2}}{m_{k}\omega_{k}^{2}}q^{2}, \qquad (1.1)$$

where the last term on the right-hand side of this equation is a counter term which has exhaustively been discussed in the literature<sup>7,8</sup> and V(q) is the external potential to which the particle is subject. The choice of the model (1.1) is partially justified in Ref. 8.

The reduced density operator of the system, in the coordinate representation, is written  $as^3$ 

$$\widetilde{\rho}(x,y,t) = \int d\mathbf{R} \langle x \mathbf{R} | \rho(t) | y \mathbf{R} \rangle$$
  
= 
$$\int \int \int \int \int dx' dy' d\mathbf{R} d\mathbf{Q}' d\mathbf{R}' K(x,\mathbf{R},t;x',\mathbf{R}',0) K^*(y,\mathbf{R},t;y',\mathbf{Q}',0) \langle x'\mathbf{R}' | \rho(0) | y'\mathbf{Q}' \rangle , \qquad (1.2)$$

where **R**, **R'**, and **Q'** are arbitrary configurations (*N*-dimensional vectors) of the environmental oscillators and K is the propagator of the particle-plus-reservoir composite system.

As one can easily see, the reduced density operator of the particle at time t depends on the total density operator at time zero. The choice made by Feynman and Vernon<sup>1,2</sup> was that the initial density operator of the composite system should factorize as

$$\rho_0(\mathbf{x}'\mathbf{R}',\mathbf{y}'\mathbf{Q}') = \widetilde{\rho}_0(\mathbf{x}',\mathbf{y}')\rho_e(\mathbf{R}',\mathbf{Q}') , \qquad (1.3)$$

where  $\tilde{\rho}_0$  refers only to the system of interest while  $\rho_e$  refers to the environment. In particular, it is always assumed that  $\rho_e$  is the equilibrium density operator of the environment. Once this is done we can write

$$\widetilde{\rho}(x,y,t) = \int \int dx' dy' J(x,y,t;x',y',0) \widetilde{\rho}_0(x',y') , \qquad (1.4)$$

where

$$J(x,y,t;x',y',0) = \int \int \int d\mathbf{R} \, d\mathbf{Q}' d\mathbf{R}' K(x,\mathbf{R},t;x',\mathbf{R}',0)$$
$$\times K^*(y,\mathbf{R},t;y',\mathbf{Q}',0)\rho_e(\mathbf{R}',\mathbf{Q}')$$
(1.5)

is a generalized "propagator" for the reduced density operator of the system. Now, using the Feynman pathintegral representation for the propagator K, the function J can be expressed as

$$J(x,y,t;x',y',0) = \int_{x'}^{x} \int_{y'}^{y} Dx(t') Dy(t') \exp\left[\frac{i}{\hbar} S_0[x(t')]\right]$$
$$\times \exp\left[-\frac{i}{\hbar} S_0[y(t')]\right]$$
$$\times \mathcal{F}[x(t'),y(t')], \quad (1.6)$$

where  $S_0[$  ] is the action of the system of interest only, while  $\mathcal{F}[$ , ], the so-called influence functional, is given by

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41 3103

$$\mathcal{F}[x(t'),y(t')] = \int \int \int d\mathbf{R} \, d\mathbf{Q}' d\mathbf{R}' \rho_e(\mathbf{R}',\mathbf{Q}') \int_{\mathbf{R}'}^{\mathbf{R}} \int_{\mathbf{Q}'}^{\mathbf{R}} D\mathbf{R}(t') D\mathbf{Q}(t') \exp\left[\frac{i}{\hbar} \{S_e[\mathbf{R}(t')] + S_I[\mathbf{R}(t'),x(t')]\}\right] \times \exp\left[-\frac{i}{\hbar} \{S_e[\mathbf{Q}(t')] + S_I[\mathbf{Q}(t'),y(t')]\}\right], \quad (1.7)$$

where  $S_{e}[]$  is the action of the environment and  $S_{I}[]$ , ] is the action of the coupling between the two systems.

This influence functional can be evaluated exactly because it is nothing but a product of propagators of harmonic oscillators subject to external forces  $(C_k q)$  averaged by the equilibrium distribution  $\rho_e$  and traced over the final configurations **R**. The result is<sup>3</sup>

$$\mathcal{F}[x(t'),y(t')] = \exp\left[\frac{i}{\hbar} \int_0^\infty d\omega \frac{J(\omega)}{\pi} \int_0^t d\tau \int_0^\tau d\sigma [x(\tau) - y(\tau)] \sin[\omega(\tau - \sigma)] [x(\sigma) + y(\sigma)]\right] \\ \times \exp\left[\frac{-1}{\hbar} \int_0^\infty d\omega \frac{J(\omega)}{\pi} \coth \frac{\hbar\omega}{2k_B T} \int_0^t d\tau \int_0^\tau d\sigma [x(\tau) - y(\tau)] \cos[\omega(\tau - \sigma)] [x(\sigma) - y(\sigma)]\right], \quad (1.8)$$

where the spectral function  $J(\omega)$  has been defined as

$$J(\omega) \equiv \frac{\pi}{2} \sum_{k} \frac{C_{k}^{2}}{m_{k}\omega_{k}} \delta(\omega - \omega_{k}) . \qquad (1.9)$$

In the case of Brownian motion  $J(\omega)$  is modeled by<sup>3</sup>

$$J(\omega) = \begin{cases} \eta \omega & \text{if } \omega < \Omega \\ 0 & \text{if } \omega > \Omega \end{cases},$$
(1.10)

where  $\Omega$  is a cutoff frequency, much larger than the natural frequencies of motion of the system of interest. However, the formulation is quite general and (1.9) can assume forms other than (1.10).

Now we are ready to study the restricted dynamics of the system of interest by solving the double path integral (1.6) together with the double convolution (1.4). Although the exact evaluation of these integrals is only possible for a restricted number of problems, there are many approximation methods available in the literature (saddle-point method, dilute gas approximation, etc.) which allows us to invest in more complicated problems.

The first attempt (successful, we must say) to write a more general form for the influence functional based on nonfactorizable initial conditions was carried forward by Hakim and Ambegaokar<sup>9</sup> who made explicit use of the translation invariance of (1.1) when V(q)=0. In this way they were able to perform some unitary transformations and, finally, diagonalize the problem exactly. Although their formulation is extremely elegant, it cannot be applied to systems which do not present any symmetry.

Recently we extended the Feynman-Vernon formulation so that it could cope with more general initial conditions, and we were able to write down a generalized expression to replace the influence functional (1.7).<sup>10</sup> The expression is more cumbersome than (1.7) and its application to arbitrary potentials involves a great deal of mathematical skill. Nevertheless, we think it is still quite useful if we wish to obtain the reduced dynamics of the particle under certain approximations.

In Sec. II we discuss the sort of initial conditions one could use instead of (1.3) while we briefly review the way

we can achieve a generalized influence functional in Sec. III.

In Sec. IV we apply the results of Sec. III to the case of the damped harmonic oscillator. In the appropriate limit of vanishing natural frequency ( $\omega_0=0$ ) we can recover the influence functional that Hakim and Ambegaokar wrote for the damped free particle. This is indeed a very reliable check for our approach.

Section V is devoted to the calculation of the function J(x,y,t;x',y',0) for the quantum Brownian oscillator while we compute the average values of observables in Sec. VI. The conclusions are presented in Sec. VII.

### **II. GENERALIZED INITIAL CONDITION**

In a recent report<sup>10</sup> the present authors generalized the method of Feynman and Vernon in order to deal with initial conditions different from (1.3). On that occasion the authors treated three new possibilities which are explained in the following.

Case (i). We have

$$\rho_0(\mathbf{x}'\mathbf{R}',\mathbf{y}'\mathbf{Q}') = \widetilde{\rho}_0(\mathbf{x}',\mathbf{y}')\rho_{eq}^{(es)}(\mathbf{x}',\mathbf{y}';\mathbf{R}',\mathbf{Q}') . \qquad (2.1)$$

Here  $\tilde{\rho}_0$  is an arbitrary function depending only on the system variables while  $\rho_{eq}^{(es)}$  stands for the equilibrium density operator of the complete "universe" formed by the system and its environment. This can be interpreted as the result of a measurement of position on the system only, once we know that the system and its environment are together in thermal equilibrium before the measuring process. To show that this physical picture really corresponds to the mathematical expression in (2.1) is not a hard matter.

Let us initially consider a pure state  $|\psi\rangle$  of the whole universe, then

$$|\psi\rangle = \int dx \, d\mathbf{R}\psi(x,\mathbf{R})|x\rangle \otimes |\mathbf{R}\rangle , \qquad (2.2)$$

where  $|\mathbf{R}\rangle = |q_1\rangle \otimes |q_2\rangle \otimes \cdots \otimes |q_N\rangle$ . A measurement of the position of the particle only can be performed by the application of the operator  $\mathcal{P}$  defined as

$$\mathcal{P} \equiv \int_{-\infty}^{\infty} dx f(x) |x\rangle \langle x| \otimes \mathcal{J}(\mathbf{R}) , \qquad (2.3)$$

where f(x) is an arbitrary function and  $\mathcal{I}(\mathbf{R})$  is the identity operator in the subspace of the environment. Let us call  $\mathcal{P}$  the measuring operator.

When we are referring to an ideal measurement,  $\mathcal{P}$  is a projection operator ( $\mathcal{P}^2 = \mathcal{P}$ ) (see Ref. 11). In this case, for a measurement of position at  $x_0$  with uncertainty  $\Delta x$ , f(x) is

$$f(x) = \Theta(x - x_0 + \Delta x/2)\Theta(x_0 + \Delta x/2 - x)$$
, (2.4)

where  $\Theta$  is the Heaviside function. The state after measurement is then<sup>11</sup>

$$|\psi_{0}\rangle = \frac{\mathcal{P}|\psi\rangle}{\sqrt{\langle\psi|\mathcal{P}|\psi\rangle}} \quad . \tag{2.5}$$

In the case of nonideal measurement, f(x) can assume any general form which is centered at  $x_0$  with width  $\Delta x$ ; for instance, a Gaussian. The difference now is that  $\mathcal{P}$  is no longer a projection operator. Therefore (2.5) must be modified to

$$|\psi_{0}\rangle = \frac{\mathcal{P}|\psi\rangle}{\left(\langle \psi|\mathcal{P}^{2}|\psi\rangle\right)^{1/2}} . \tag{2.6}$$

Since this is more general than (2.5) we shall only use it

All of what we have been saying can be generalized for the case when the "universe" is no longer in a pure state but is in a statistical mixture instead. Let us consider the whole universe initially in thermal equilibrium. Then

$$\rho = \sum_{n, \{n_i\}} e^{-\beta E_{n\{n_i\}}} |\psi_{n\{n_i\}}\rangle \langle \psi_{n\{n_i\}}| , \qquad (2.7)$$

where  $\{n_i\}$  stands for the set of N quantum numbers  $\{n_1, n_2, \ldots, n_N\}$  for the reservoir oscillators, and  $|\psi_{n\{n_i\}}\rangle$  is an eigenstate of the composite system. Equation (2.7) can further be written as

$$\rho = \sum_{n_i \{n_i\}} e^{-\beta \mathcal{E}_{n \{n_i\}}} \int \int \int \int dx \, dx' d\mathbf{R} \, d\mathbf{R}' \psi_{n \{n_i\}}(x, \mathbf{R})$$
$$\times \psi_{n \{n_i\}}^*(x', \mathbf{R}')$$
$$\times |x\rangle \langle x'| \otimes |\mathbf{R}\rangle \langle \mathbf{R}'| . \quad (2.8)$$

Now, just after measurement the density operator of the universe can be written  $as^{11}$ 

$$\rho_0 = \frac{\mathcal{P}\rho\mathcal{P}}{\mathrm{tr}\mathcal{P}^2\rho} , \qquad (2.9)$$

which is a generalization of (2.6) for the case of mixtures. Now using (2.3) for  $\mathcal{P}$  we have

$$\rho_{0} = \left[ \sum_{n, \{n_{i}\}} e^{-\beta E_{n\{n_{i}\}}} \int \int \int dx \, dx' d\mathbf{R} \, d\mathbf{R}' f(x) f(x') \psi_{n\{n\}_{i}}(x, \mathbf{R}) \psi_{n\{n\}_{i}}^{*}(x', \mathbf{R}') \\ \times |x\rangle \langle x'| \otimes |\mathbf{R}\rangle \langle \mathbf{R}'| \right] / \left[ \sum_{n\{n_{i}\}} e^{-\beta E_{n\{n_{i}\}}} \int \int dx \, d\mathbf{R} \, f(x)^{2} |\psi_{n\{n\}_{i}}(x, \mathbf{R})|^{2} \right], \quad (2.10)$$

which finally implies that

$$\rho_{0}(x',\mathbf{R}';y',\mathbf{Q}') = \frac{f(x')f(y')\rho_{eq}^{(es)}(x',\mathbf{R}';y',\mathbf{Q}')}{\int \int dx \, d\mathbf{R} \, f(x)^{2}\rho_{eq}^{(es)}(x,\mathbf{R};x,\mathbf{R})} \,.$$
(2.11)

Now, comparing (2.11) with (2.1) allows us to identify

$$\widetilde{\rho}_{0}(\mathbf{x}',\mathbf{y}') = \frac{f(\mathbf{x}')f(\mathbf{y}')}{\int \int d\mathbf{x} \, d\mathbf{R} \, f(\mathbf{x})^{2} \rho_{\text{eq}}^{(es)}(\mathbf{x},\mathbf{R};\mathbf{x},\mathbf{R})} \qquad (2.12)$$

as a function of the system of variables which depends only on the measuring (or preparation) procedure.

Case (ii). We have

$$\rho_0(\mathbf{x}'\mathbf{R}',\mathbf{y}'\mathbf{Q}') = \overline{\rho}_{eq}^{(es)}(\mathbf{x}',\mathbf{y}';\mathbf{R}',\mathbf{Q}') . \qquad (2.13)$$

Here,  $\bar{\rho}_{eq}^{(es)}$  is the equilibrium density operator of the universe when the particle is subject to a potential  $\bar{V}(q)$ which is abruptly modified to V(q) at t=0. When this modification takes place  $\bar{\rho}_{eq}^{(es)}$  is no longer an equilibrium state of the "universe." Consequently, it relaxes to a new equilibrium state  $\rho_{eq}^{(es)}(x,y;\mathbf{R},\mathbf{Q})$  which is the equilibrium state of the universe when the particle of interest is subject to V(q). We shall call  $\bar{V}(q)$  the preparation potential. Case (iii). We have

$$\rho_0(\mathbf{x}'\mathbf{R}',\mathbf{y}'\mathbf{Q}') = \widetilde{\rho}_0(\mathbf{x}',\mathbf{y}')\overline{\rho}_{eq}^{(es)}(\mathbf{x}',\mathbf{y}';\mathbf{R}',\mathbf{Q}') . \qquad (2.14)$$

This case is a combination of the previous ones. At t=0 the particle of interest is subject to a preparation potential  $\overline{V}(q)$ . Then we perform a measurement on the position of the particle only and simultaneously change the preparation potential to V(q). This new state is not even an equilibrium state of the universe when the particle is subject to  $\overline{V}(q)$ . If we trace back all the steps that led us to (2.12) one can easily convince oneself that now

$$\tilde{\rho}_0(x',y') = \frac{f(x')f(y')}{\int \int dx \, d\mathbf{R} \, f(x)^2 \bar{\rho}_{eq}^{(es)}(x,\mathbf{R};x,\mathbf{R})} \quad (2.15)$$

Since this last case includes cases (i) and (ii) we shall develop the new influence functional only for case (iii) and particularize it to (i) or (ii) whenever necessary.

Finally we wish to mention that f(x) could be the result of a succession of measurements. For instance, it could represent the result of the measurement of position with uncertainty  $\Delta x$  and a later measurement of momentum with uncertainty  $\Delta p$ . In this case f(x) is a complex function (for example, a Gaussian of width  $\Delta x$  centered at  $x_0$  multiplied by a plane wave with wave vector  $p_0/\hbar$ ).

# **III. THE NEW INFLUENCE FUNCTIONAL (NIF)**

In this section it is our intention to briefly review the obtainment of the influence functional once we have avoided the factorizable initial condition. Although this has already been done in a separate report<sup>10</sup> we think the general idea should be repeated here for the sake of com-

pleteness. However, we shall try to make it quite brief in order to avoid unnecessary overlap with our previous work.

In this new situation the reduced density operator of the particle can still be written in the form (1.4). The difference is that J must now be written as

$$J(x,y,t;x',y',0) = \int_{x'}^{x} \int_{y'}^{y} Dx(t') Dy(t') \exp\left[\frac{i}{\hbar} \tilde{S}_{0}[x(t')]\right] \exp\left[-\frac{i}{\hbar} \tilde{S}_{0}[y(t')]\right] F([x],[y],x',y'), \qquad (3.1)$$

where

$$F = \int \int \int d\mathbf{R} \, d\mathbf{Q}' d\mathbf{R}' \overline{\rho}_{\text{eq}}^{(es)}(\mathbf{x}', \mathbf{R}'; \mathbf{y}', \mathbf{Q}') G([\mathbf{x}], [\mathbf{y}], \mathbf{R}, \mathbf{R}', \mathbf{Q}')$$
(3.2)

and

$$G = \int_{\mathbf{R}'}^{\mathbf{R}} \int_{\mathbf{Q}'}^{\mathbf{R}} D\mathbf{R}(t') D\mathbf{Q}(t') \exp\left[\frac{i}{\hbar} \{S_e[\mathbf{R}(t')] + S_I[\mathbf{R}(t'), \mathbf{x}(t')]\}\right] \exp\left[-\frac{i}{\hbar} \{S_e[\mathbf{Q}(t')] + S_I[\mathbf{Q}(t'), \mathbf{y}(t')]\}\right] .$$
(3.3)

In our notation, variables within brackets are paths connecting the appropriate end points (variables without brackets) and D (variable) is the properly normalized variation of those paths. The tilde upon the action  $S_0$  means that the counterterm is included therein.

The path integral (3.3) is a standard one,<sup>2,12</sup> since it is the product of propagators of forced harmonic oscillators. On the other hand, the equilibrium density operator  $\bar{\rho}_{eq}^{(es)}$  has the path-integral representation

$$\bar{\rho}_{eq}^{(es)}(x',\mathbf{R}';y',\mathbf{Q}') = \int_{y'}^{x'} Dz(t') \exp(-\bar{\tilde{S}}_{0}^{(E)}[z]/\hbar) G^{(E)}(\mathbf{R}',\mathbf{Q}',[z]) , \qquad (3.4)$$

where

$$G^{(E)}(\mathbf{R}',\mathbf{Q}',[z]) = \prod_{\alpha} \int_{\mathcal{Q}'_{\alpha}}^{\mathcal{R}'_{\alpha}} D\widetilde{R}_{\alpha} \exp\left[-\frac{1}{\hbar} (S_{I}^{(E)}[z,\widetilde{R}_{\alpha}] + S_{e}^{(E)}[\widetilde{R}_{\alpha}])\right]$$
(3.5)

and  $S^{(E)}$  is the Euclidean version of the corresponding action which means that we must replace all the potentials (including the interaction) by minus its value. The bar on top of  $S_0^{(E)}$  means that the potential on the particle is the preparation potential  $\overline{V}(q)$ . Here too, (3.5) is a product of integrals of forced harmonic oscillators. Therefore, combining the results of (3.3) and (3.5) (see Ref. 10) one can show that the NIF can be written as

$$F([x],[y],x',y') = \mathcal{F}[x,y] \int_{y'}^{x'} Dz(u') \exp\left[-\frac{1}{\hbar} \overline{S}_{0}^{(E)}[z]\right]$$

$$\times \exp\left[\frac{-1}{4\pi\hbar} \int_{0}^{U} du \int_{-\infty}^{\infty} du' \int_{0}^{\infty} d\omega J(\omega) \exp(-\omega|u-u'|) \times [z(u)-z(u')]^{2} \exp\left[\frac{-1}{\hbar} \int_{0}^{U} z(u)f(u) du\right], \quad (3.6)$$

where

$$f(u) = \frac{-1}{\pi} \int_0^t dt' [x(t') - y(t')] \int_0^\infty d\omega J(\omega) \sin\omega t' [\coth(\omega U/2) \sinh(\omega u) - \cosh(\omega u)] - \frac{i}{\pi} \int_0^t dt' [x(t') - y(t')] \int_0^\infty d\omega J(\omega) \cos\omega t' [\coth(\omega U/2) \cosh(\omega u) - \sinh(\omega u)].$$
(3.7)

 $\mathcal{F}[x,y]$  is the FV influence functional as obtained in (1.8) and  $U = \hbar\beta$ .

We can now define another functional  $\mathcal{F}_T$  as

$$\mathcal{F}_{T}[x,y,z] = \mathcal{F}[x,y] \exp\left[\frac{-1}{4\pi\hbar} \int_{0}^{U} du \int_{-\infty}^{\infty} du' \int_{0}^{\infty} d\omega J(\omega) \exp(-\omega|u-u'|) [z(u)-z(u')]^{2}\right] \exp\left[\frac{-1}{\hbar} \int_{0}^{U} z(u) f(u) du\right],$$
(3.8)

in such a way that

$$J(x,y,t;x',y',0) = \int_{x'}^{x} \int_{y'}^{y} \int_{y'}^{x'} Dx(t') Dy(t') Dz(u') \mathcal{F}_{T}[x,y,z] \exp\left[\frac{i}{\hbar} \widetilde{S}_{0}[x(t')]\right] \times \exp\left[-\frac{i}{\hbar} \widetilde{S}_{0}[y(t')]\right] \exp\left[-\frac{1}{\hbar} \overline{S}_{0}^{(E)}[z]\right].$$
(3.9)

Once again we emphasize that in  $\tilde{S}_0$  the potential is V(q) plus the counterterm, while in  $\bar{S}_0^{(E)}$  the potential is  $\bar{V}(q)$  and the counterterm has already been eliminated. For the particular case of the initial condition (i) we must replace  $\bar{S}_0^{(E)}$  by  $S_0^{(E)}$  and apply (3.9) in (1.4). For case (ii), (3.9) must be used in (1.4) without  $\tilde{\rho}_0(x',y')$ .

It is worth noting that together with  $\mathcal{F}[x,y]$  (which carries a sort of retarded and advanced coupling between paths running forward and backward in time) there appears in (3.8) two new terms—one which represents a self-interaction of a thermal path and another which couples the thermal path z(u) to the dynamical paths x(t') and y(t').

### IV. THE NIF FOR THE HARMONIC OSCILLATOR

In order to apply (3.9) to a specific example let us choose one of the initial conditions proposed in Sec. II;

where

$$S_{\text{eff}}[z] \equiv \bar{S}_{0}^{E}[z] + \frac{\eta}{4\pi} \int_{-\infty}^{\infty} du' \int_{0}^{U} du \int_{0}^{\infty} d\omega \, \omega [z(u) - z(u')]^{2} \exp(-\omega |u - u'|) + \frac{1}{\pi} \int_{0}^{U} du \, f(u) z(u)$$
(4.2)

and f(u) has previously been defined in (3.7). By (3.6) we obviously have

$$F([x],[y],x',y') = \mathcal{F}[x,y]I([x],[y],x',y') .$$
(4.3)

The effective action in (4.2) is a functional of z(u) which has a quadratic and a linear term in this variable. Therefore (4.1) is the kind of functional integral that can (at least, in principle) be solved exactly by a simple method. All we must do is to take the first functional derivative of  $S_{\text{eff}}$  and find out the path  $z_c$  that extremizes the effective action. This means

$$\frac{\delta S_{\text{eff}}}{\delta z(u)} \bigg|_{z=z_c(u)} = 0 .$$
(4.4)

Once this has been done we must evaluate the second functional derivative of  $S_{\text{eff}}$  at  $z_c(u)$  and solve the resulting eigenvalue problem

$$\int \frac{\delta^2 S_{\text{eff}}}{\delta z(u) \, \delta z(u')} \bigg|_{z=z_c(u)} \delta z(u') \, du' = \lambda \, \delta z(u) \, . \tag{4.5}$$

The final result for (4.1) is then

$$I([x],[y],x',y') = \mathcal{N}\left[\frac{1}{\prod_{\alpha}\lambda_{\alpha}}\right]^{1/2} \exp\left[\frac{-1}{\hbar}S_{\text{eff}}[z_{c}]\right],$$

where  $\mathcal{N}$  is a normalization constant and  $\{\lambda_{\alpha}\}$  is the set of eigenvalues of (4.5).

we shall take case (i) ( $\overline{V} = V$ ). Then we need to evaluate a

First we will evaluate the path integral in z(u) and then the resulting integral (3.1) following the same pro-

cedure as in (3.9). In other words, we must first evaluate

the path integral that appears multiplying  $\mathcal{F}[x,y]$  in (3.6) (with  $\overline{S}_{0}^{(E)}$  replaced by  $S_{0}^{(E)}$ ). Another point we want to

mention is that we shall deal explicitly with Ohmic dissi-

 $I([x],[y],x',y') \equiv \int_{y'}^{x'} Dz(u') \exp\left[\frac{-1}{\hbar} S_{\text{eff}}[z(u')]\right],$ 

triple path integral and this we shall do in steps.

pation that means  $J(\omega) = \eta \omega$ .

In this way, we want to evaluate

Although these steps seem really simple this is not what happens in practice. The difficulty starts with the solution of (4.4). This is an inhomogeneous linear integro-differential equation which is not simple to solve. Therefore, we shall try to evaluate (4.1) by a slightly different method.

In the following we shall apply to this problem the same method that was developed in Ref. 8 (Appendix B) for dealing with a very similar path integral [actually the same, except for the absence of the forcing term f(u)].

The method consists of making a periodic extension of any function g(u) defined within the interval (0, U). Then we can write the periodic extension of z(u) or f(u)as a Fourier series and express  $S_{\text{eff}}[z]$  as a function of the Fourier coefficients of z(u) and f(u).

The next step is to extremize  $S_{\text{eff}}[z]$  subject to the boundary conditions on z(u), namely, z(0)=y' and z(U)=x'. These two equations can also be written in terms of the above-mentioned Fourier coefficients and, consequently, be regarded as constraints for our variational problem. This is a standard problem of Lagrange multipliers. Therefore, following the results of Appendix A we can write [see (4.6)]

$$I([q],[\xi],q',\xi') = I_0(t) \exp(-\bar{S}_{\rm eff}/\hbar) , \qquad (4.7)$$

(4.6) where

(4.1)

$$\overline{S}_{\text{eff}} = \frac{\eta}{2\pi} \int_{0}^{\Omega} d\omega \frac{\omega^{3} \coth(\omega U/2)}{(\omega_{0}^{2} - \omega^{2})^{2} + 4\gamma^{2} \omega^{2}} \left[ (\xi')^{2} - \xi' \int_{0}^{t} dt' \xi(t') \left[ \frac{2(\omega^{2} - \omega_{0}^{2})}{\omega} \sin\omega t' - \frac{2\eta}{M} \cos\omega t' \right] \right]$$

$$+ \frac{M}{2\kappa} \left[ q' + \frac{2i\gamma}{\pi} \int_{0}^{t} dt' \int_{0}^{\Omega} d\omega \frac{\omega \coth(\omega U/2)}{(\omega_{0}^{2} - \omega^{2})^{2} + 4\gamma^{2} \omega^{2}} \xi(t') \left[ (\omega_{0}^{2} - \omega^{2}) \cos\omega t' - \frac{\eta}{M} \omega \sin\omega t' \right] \right]^{2} - i\eta q' \xi'$$

$$(4.8)$$

with the new paths  $\xi(t')$  and q(t') defined as

$$\xi(t') \equiv x(t') - y(t'), \quad q(t') \equiv \frac{x(t') + y(t')}{2} \quad . \tag{4.9}$$

Notice that  $\overline{S}_{\text{eff}}$  is a functional of  $\xi(t')$  and a function of  $\xi'$  and q'. The new influence functional can now be written as

$$F([x], [y], x', y') = I_0(t) \mathcal{F}[x, y] \exp(-\bar{S}_{\text{eff}} / \hbar) , \quad (4.10)$$

where  $I_0(t)$  is the result of the Gaussian path integral one has to solve with the second functional derivative of  $S_{\text{eff}}$ . Nevertheless, we shall not evaluate this integral explicitly and leave  $I_0(t)$  to be computed by the normalization of the final form of the reduced density operator.

Before we write a final expression for F([x], [y], x', y')let us briefly analyze  $\overline{S}_{eff}$ . This action contains a real and an imaginary part. If we take the limit  $\omega_0 \rightarrow 0$  we easily recover the result of Ref. 9. In this limit,  $\kappa$  (which is equal to  $\langle q^2 \rangle$  in equilibrium) tends to infinity and we end up with the same correction Hakim and Ambegaokar found to the old influence functional.

Another interesting limit is when we neglect the time dependence in (4.8)  $[\xi(t')=0]$ . That expression then becomes, as it should, the exponent of the reduced density operator of the oscillator in equilibrium with its environment (see Appendix B of Ref. 8).

In order to close this section let us write the new influence functional in terms of the newly defined paths  $\xi(t')$  and q(t'). Using (4.9) in (1.8) and evaluating the frequency integrals for the imaginary part of the exponent of  $\mathcal{F}$  [for  $J(\omega)$  given by (1.10)] we get (see Ref. 3 for details)

$$\operatorname{Im} \ln \mathcal{F} = \frac{2\eta \Omega}{\pi} \int_0^t \xi(t') q(t') dt' - \eta q' \xi' -\eta \int_0^t \xi(t') \dot{q}(t') dt' , \qquad (4.11)$$

and then

$$F([q],[\xi],q',\xi') = I_0(t) \exp\left[\frac{i}{\hbar} \left[\frac{2\eta\Omega}{\pi} \int_0^t \xi(t')q(t')dt' - \eta q'\xi' - \eta \int_0^t \xi(t')\dot{q}(t')dt'\right]\right] \exp\left[\frac{-1}{\hbar}\overline{S}_{\text{eff}}([\xi],\xi'q')\right].$$
(4.12)

Finally, we see that the second term inside the brackets in (4.12) identically cancels the last term on the right-hand side of (4.8). This term in (4.12) had been neglected in Ref. 3 by a wrong argument. Now, it is clear that after changing the initial conditions, this term naturally disappears.

tion  $J(q,\xi,t;q',\xi',0)$ . Substituting (4.10) in (3.1) and changing variables to  $q(t'),\xi(t')$  we have

$$J(q,\xi,t;q',\xi',0) = I_0(t) \int_{q'}^{q} \int_{\xi'}^{\xi} Dq(t') D\xi(t') \exp\left[\frac{iS_1 - S_2 - S_3}{\hbar}\right],$$
(5.1)

### V. THE FUNCTION $J(q, \xi, t; q', \xi', 0)$

Once we have computed  $F([q],[\xi],q',\xi')$  we can write directly the double path integral representing the func-

where

$$S_{1} = \int_{0}^{t} dt' [M\dot{q}(t')\dot{\xi}(t') - M\omega_{0}^{2}q(t')\xi(t') - \eta\dot{q}(t')\xi(t')], \qquad (5.2)$$

$$S_{2} = \frac{\eta}{2\pi} \int_{0}^{\Omega} d\omega \,\omega \coth(\omega U/2) \int_{0}^{t} dt' \int_{0}^{t} dt'' \xi(t') \xi(t'') \cos\omega(t'-t'') \\ + \frac{\eta}{2\pi} \int_{0}^{\Omega} d\omega \frac{\omega^{3} \coth(\omega U/2)}{(\omega_{0}^{2}-\omega^{2})^{2}+4\gamma^{2}\omega^{2}} \left[ (\xi')^{2} - \xi' \int_{0}^{t} dt' \xi(t') \left[ \frac{2(\omega^{2}-\omega_{0}^{2})}{\omega} \sin\omega t' - \frac{2\eta}{M} \cos\omega t' \right] \right],$$
(5.3)

$$S_{3} = \frac{MU}{2\kappa} \left[ q' + \frac{2i\gamma}{\pi} \int_{0}^{t} dt' \int_{0}^{\Omega} d\omega \frac{\omega \coth(\omega U/2)}{(\omega_{0}^{2} - \omega^{2})^{2} + 4\gamma^{2} \omega^{2}} \xi(t') \left[ (\omega_{0}^{2} - \omega^{2}) \cos \omega t' - \frac{\eta}{M} \omega \sin \omega t' \right] \right]^{2}.$$
(5.4)

Notice that the first term inside the brackets in (4.12) identically canceled the counterterm pieces in  $\tilde{S}_0[x]$  and  $\tilde{S}_0[y]$ .

A quick look at the expressions above will show us that the only functional of q(t') is the action  $S_1$  in (5.2). Moreover, integration by parts of the first and last terms of  $S_1$  leads us to

$$S_{1} = Mq\dot{\xi} - Mq'\dot{\xi}' - \eta q\xi + \eta q'\xi' - \int_{0}^{t} dt'q(t') [M\ddot{\xi}(t') - \eta\dot{\xi}(t') + M\omega_{0}^{2}\xi(t')] .$$
(5.5)

Therefore, the path integration on q(t') can be done by using the integral form of the  $\delta$  function

$$\int Dq(t') \exp\left[\frac{-i}{\hbar} \int_0^t dt' q(t') [\dots]\right] \propto \delta(\dots) , \qquad (5.6)$$

which allows us to trivially integrate on  $D\xi(t')$ . The result of (5.1) is simply the integrand evaluated at  $\xi_c(t')$  given by

$$M\ddot{\xi}_{c}(t') - \eta\dot{\xi}_{c}(t') + M\omega_{0}^{2}\xi_{c}(t') = 0$$
(5.7)

with boundary conditions  $\xi(0) = \xi'$  and  $\xi(t) = \xi$ .

Let us particularize our application to the underdamped harmonic oscillator ( $\omega_0 > \gamma$ ). Then

$$\xi_c(t') = \frac{1}{\operatorname{sinv}t} [\xi e^{-\gamma t} \operatorname{sinv}t' + \xi' \operatorname{sinv}(t-t')] e^{\gamma t'}, \qquad (5.8)$$

where

$$v \equiv (\omega_0^2 - \gamma^2)^{1/2} . \tag{5.9}$$

When  $\gamma > \omega_0$  we must replace  $\nu \rightarrow i (\gamma^2 - \omega_0^2)^{1/2}$  (overdamped harmonic oscillator) while when  $\omega_0 = 0$  (free particle) one respaces  $\nu \rightarrow i \gamma$ .

The procedure is now straightforward. We just evaluate the integrand at  $\xi_c$  and collect the resulting terms in an appropriate form. The result after this simple (but tedious) job is

$$J(q,\xi,t;q',\xi',0) = I_0 \exp\left\{\frac{i}{\hbar} \left[ \left[K(t) - M\gamma\right]q\xi + \left[K(t) + M\gamma - \frac{MUE(t)}{\kappa}\right]q'\xi' - N(t)q\xi' - \left[A(t) - \frac{MUD(t)^2}{2\kappa}\right]\xi^2 - \left[\frac{MUD(t)}{\kappa} + L(t)\right]q'\xi\right] \right\} \exp\left\{\frac{-1}{\hbar} \left[ \left[\frac{MU}{2\kappa}\right](q')^2 + \left[A(t) - \frac{MUD(t)^2}{2\kappa}\right]\xi^2 + \left[B(t) - \frac{MUD(t)E(t)}{\kappa}\right]\xi\xi' + \left[C(t) - \frac{MUE(t)^2}{2\kappa}\right](\xi')^2\right] \right\}, \quad (5.10)$$

where

 $K(t) \equiv M v \operatorname{cotan} v t$ ,

$$N(t) = \frac{M v e^{\gamma t}}{\sin v t} , \qquad (5.12)$$

$$L(t) \equiv \frac{M v e^{-\gamma t}}{\sin v t} , \qquad (5.13)$$

and A(t), B(t), C(t), D(t), and E(t) are of the form

$$f(t) = \frac{M\gamma}{\pi} \int_0^{\Omega} d\omega \,\omega \coth(\omega U/2) f_{\omega}(t) , \qquad (5.14)$$

with

$$A_{\omega}(t) = \frac{e^{-2\gamma t}}{\sin^2 \nu t} \int_0^t dt' \int_0^t dt'' \sin\nu t' \cos\omega (t'-t'') \sin\nu t'' e^{\gamma (t'+t'')} , \qquad (5.15)$$

$$B_{\omega}(t) = \frac{2e^{-\gamma t}}{\sin^{2}\nu t} \int_{0}^{t} dt' \int_{0}^{t} dt'' \sin\nu t' \cos\omega(t'-t'') \sin\nu(t-t'') e^{\gamma(t'+t'')} + \frac{4\gamma\omega^{2}}{(\omega_{0}^{2}-\omega^{2})^{2}+4\gamma^{2}\omega^{2}} \frac{e^{-\gamma t}}{\sin\nu t} \int_{0}^{t} dt' \sin\nu t' \cos\omega t' e^{\gamma t'} + \frac{4\gamma\omega^{2}}{(\omega_{0}^{2}-\omega^{2})^{2}+4\gamma^{2}\omega^{2}} \frac{e^{-\gamma t}}{\sin\nu t} \int_{0}^{t} dt' \sin\nu t' \sin\omega t' e^{\gamma t'} ,$$
(5.16)

(5.11)

$$C_{\omega}(t) = \frac{1}{\sin^{2}\nu t} \int_{0}^{t} dt' \int_{0}^{t} dt'' \sin\nu(t-t') \cos\omega(t'-t'') \sin\nu(t-t'') e^{\gamma(t'+t'')} + \frac{4\gamma\omega^{2}}{(\omega_{0}^{2}-\omega^{2})^{2}+4\gamma^{2}\omega^{2}} \frac{1}{\sin\nu t} \int_{0}^{t} dt' \sin\nu(t-t') \cos\omega t' e^{\gamma t'} - \frac{2\omega(\omega^{2}-\omega_{0}^{2})}{(\omega_{0}^{2}-\omega^{2})^{2}+4\gamma^{2}\omega^{2}} \frac{1}{\sin\nu t} \int_{0}^{t} dt' \sin\omega t' \sin\nu(t-t') e^{\gamma t'} + \frac{\omega^{2}}{(\omega_{0}^{2}-\omega^{2})^{2}+4\gamma^{2}\omega^{2}} ,$$
(5.17)

$$D_{\omega}(t) = \frac{2e^{-\gamma t}}{M \operatorname{sinv}t} \frac{1}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2 \omega^2} \int_0^t dt' \operatorname{sinv}t' e^{\gamma t'} \left[ (\omega_0^2 - \omega^2) \cos \omega t' - \frac{\eta \omega}{M} \sin \omega t' \right],$$
(5.18)

$$E_{\omega}(t) = \frac{2}{M \operatorname{sinv}t} \frac{1}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2 \omega^2} \int_0^t dt' \operatorname{sinv}(t - t') e^{\gamma t'} \left[ (\omega_0^2 - \omega^2) \cos \omega t' - \frac{\eta \omega}{M} \sin \omega t' \right].$$
(5.19)

At this point it is interesting to compare our results with the previous ones obtained in the case of factorizable initial conditions.<sup>3</sup> Expression (5.10) is of the same form as before; the difference lies in the functions from B(t) to E(t). Our new K(t), L(t), N(t), and A(t) are exactly the same as in Ref. 3. For the case of factorizable initial conditions,  $B_{\omega}(t)$  and  $C_{\omega}(t)$  contain only the first integrals in (5.16) and (5.17) while  $D_{\omega}(t)$  and  $E_{\omega}(t)$  do not exist.

Finally, let us compute the term  $I_0(t)$  to complete the evaluation of  $J(q,\xi,t;q',\xi',0)$ . This can be easily done by normalizing the reduced density operator  $\tilde{\rho}(q,\xi,t)$  of the oscillator, as we show in Appendix B. We find

$$I_0(t) = \frac{N(t)}{2\pi\hbar}$$
 (5.20)

# VI. THE AVERAGE VALUES OF OBSERVABLES

For a generic function of position, say F(q), we have

$$\langle F(q) \rangle_t = \int dq \ F(q) \widetilde{\rho}(q, \xi = 0, t)$$
 (6.1)

On the other hand, we have shown that  $\tilde{\rho}(q,\xi=0,t)$  can be written as

$$\widetilde{\rho}(q,0,t) = \frac{N(t)}{2\pi\hbar} \int \int dq' d\xi' \widetilde{\rho}_0(q',\xi') \widetilde{J}(q,0,t;q',\xi',0) ,$$
(6.2)

where  $\tilde{J}$  can be identified as [see (5.10)]

$$\widetilde{J}(q,0,t;q',\xi',0) = \exp\left[\frac{i}{\hbar}[\alpha(t)q'\xi' - N(t)q\xi'\right] \\ \times \exp\left[\frac{-1}{\hbar}\left[\frac{(q')^2}{2\lambda} + \Delta(t)(\xi')^2\right]\right],$$
(6.3)

with the newly defined functions

$$\alpha(t) \equiv K(t) + M\gamma - MUE(t)/\kappa , \qquad (6.4)$$

$$\lambda \equiv \kappa / M U , \qquad (6.5)$$

$$\Delta(t) \equiv C(t) - E(t)^2 / 2\lambda . \qquad (6.6)$$

Noticing that the only dependence on q comes from the second term in the first exponential of (6.3) we can readily evaluate the integral over q which results in

$$\int dq F(q) \exp\left[\frac{-i}{\hbar}N(t)q\xi'\right]$$
$$= \int dq F\left[\frac{i\hbar}{N(t)}\frac{\partial}{\partial\xi'}\right] \exp\left[\frac{-i}{\hbar}N(t)q\xi'\right]$$
$$= F\left[\frac{i\hbar}{N(t)}\frac{\partial}{\partial\xi'}\right]\frac{2\pi\hbar}{N(t)}\delta(\xi'). \quad (6.7)$$

Substituting this result in (6.1) we get

1.5

$$\langle F(q) \rangle_{t} = \int dq' \int d\xi' \left[ F\left(\frac{i\hbar\partial}{N(t)\partial\xi'}\right) \delta(\xi') \right] \exp\left(\frac{i}{\hbar}\alpha(t)q'\xi'\right) \exp\left[\frac{-1}{\hbar}\left(\frac{(q')^{2}}{2\lambda} + \Delta(t)(\xi')^{2}\right)\right] \widetilde{\rho}_{0}(q',\xi') .$$
(6.8)

For the particular cases F(q)=q and  $F(q)=q^2$  we can integrate (6.8) by parts and the final result is

$$\langle q \rangle_t = \frac{1}{N(t)} \{ [K(t) + M\gamma - E(t)/\lambda] \langle q \rangle_0 + \langle p \rangle_0 \}$$
 (6.9)

$$\langle q^2 \rangle_t = \frac{\alpha(t)}{N(t)^2} \langle qp + pq \rangle_0 + \frac{2\hbar\Delta(t)}{N(t)^2} + \frac{1}{N(t)^2} \langle p^2 \rangle_0 + \frac{\alpha(t)^2}{N(t)^2} \langle q' \rangle^2 .$$
(6.10)

Now, comparing (6.9) with the solution of the classical underdamped harmonic oscillator when  $q(0)=q_0$  and

and

 $p(0) = p_0$  that reads

$$q(t) = q_0 \cos v t e^{-\gamma t} + (q_0 \gamma / v) \sin v t e^{-\gamma t} + (p_0 / M v) \sin v t e^{-\gamma t}, \qquad (6.11)$$

we find that the only difference between these two expressions is a term proportional to  $[E(t)/\lambda N(t)]\langle q \rangle_0$ .

At first sight this term looks wrong but it can be understood as the influence of the specific preparation of the system at t=0 on its subsequent motion. Actually, one could think of it as a peculiarity of the model we have employed for the reservoir. We shall return to this point in Sec. VII.

Another important result is that  $\langle q^2 \rangle_t$  in (6.10) obeys the fluctuation-dissipation theorem when  $t \to \infty$  exactly as it happened in Ref. 3 for the case of the factorizable initial condition. However, one should notice that its time dependence is also influenced by terms dependent on the preparation procedure.

The average values of arbitrary functions of the momentum operator F(p) can also be computed in a way similar to what has been done for F(q). The starting point is now

$$\langle F(p) \rangle_t = \int dq F\left[\frac{\hbar}{i} \frac{\partial}{\partial \xi}\right] \widetilde{\rho}(q,\xi,t) \bigg|_{\xi=0}$$
 (6.12)

Then, using (6.2) and (6.3) one will be able to compute average values such as  $\langle p \rangle_t$  and  $\langle p^2 \rangle_t$ . For example,  $\langle p \rangle_t$  is given by

$$\left\langle p \right\rangle_{t} = \left[ \frac{\alpha(t) [K(t) - M\gamma]}{N(t)} - \left[ \frac{D(t)}{\lambda} + L(t) \right] \right] \left\langle q \right\rangle_{0} + \frac{[K(t) - M\gamma]}{N(t)} \left\langle p \right\rangle_{0}.$$
(6.13)

Here, too, the solution differs from its classical equivalent by terms proportional to  $D(t)\langle q \rangle_0$  and  $E(t)\langle q \rangle_0$ . Once again this is a trace of the influence of the preparation process on the dynamics of the Brownian particle. In the case of the factorizable initial condition the functions D(t) and E(t) simply do not show up and consequently  $\langle q \rangle_t$  and  $\langle p \rangle_t$  obviously coincide with their classical equivalents.

Although the evaluation of  $\langle p^2 \rangle_t$  is not difficult, the final result is quite lengthy to be explicitly written down here. The important point is that the physics contained therein is in agreement with our conclusions for the behavior of  $\langle q^2 \rangle_t$ .

Just before we leave this section we should say something about the free-particle dynamics. Taking the limit  $\omega_0 \rightarrow 0$  we can reproduce exactly all the results of Ref. 9. The reason for this is very simple. If we look at our expression (5.4) we will notice that  $S_3$  depends on  $\kappa$ . However, since  $\kappa$  is proportional to  $\langle q^2 \rangle_{eq}$  it blows up when  $\omega_0$  vanishes and we easily recover the influence functional of Hakim and Ambegaokar. Consequently, all the average values computed in Ref. 9 are the same we could compute here for  $\omega_0=0$ .

#### **VII. CONCLUSIONS**

There are two main points we would like to emphasize in this section. The first one shows why it is advantageous to consider a nonfactorizable initial condition while the second deals with the long-time decay of the initial preparation when the generalized initial condition is used.

Using the nonfactorizable initial condition we have explicitly shown that some spurious terms which have been neglected in Ref. 3 naturally disappear [see the argument just below (4.12)]. In Ref. 3 this sort of term has been neglected but the reason why this has been done is not correct. Actually, one could argue that terms like (A11) should be neglected but the reasoning would be entirely different. Since they involve integrals of a  $\delta$  function at t=0 and we are interested in time scales longer than  $\Omega^{-1}$  we should interpret those integrals as being evaluated from  $t'=0^+$  to t'=t. On the other hand, for times shorter than  $\Omega^{-1}$  the expression (A9) is continuous and in the limit  $t \rightarrow 0$  we can recover the boundary condition

$$\lim_{t \to 0} J(x, y, t; x', y', 0) = \delta(x - x')\delta(y - y') .$$
(7.1)

Another advantage of dealing with the generalized initial state is that there is no more slowly decaying terms in the dynamics of the Brownian particle which depend on the cutoff  $\Omega$ . An example of this is the time dependence of the width of the wave packet of a damped free particle. When we use the factorizable initial condition the longtime behavior of  $\langle q^2(t) \rangle$  is given by (at T=0)

$$\langle q^2(t) \rangle \approx \ln \sqrt{\gamma \Omega/2} t$$
 (7.2)

while it can be shown that for the nonfactorizable case  $\langle q^2(t) \rangle$  behaves as<sup>9</sup>

$$\langle q^2(t) \rangle \approx \ln \gamma t$$
 (7.3)

Nevertheless, there is something that worries the reader when the generalized FV is applied, namely, the presence of terms that make  $\langle q(t) \rangle$  or  $\langle p(t) \rangle$  deviate from their classical equivalents. It is our intention now to show that these terms are really expected if we consider a model Lagrangian as (1.1) even in the classical limit.

If we write down the equations of motion for q and  $q_k$ in (1.1), take the Laplace transform of all of them, and use (1.9) and (1.10) we can show that the effective equation of motion for q(t) is

$$\begin{aligned} M\ddot{q} + \eta\dot{q} + V'(q) \\ &= \frac{1}{2\pi i} \int_{\epsilon - i\infty}^{\epsilon + i\infty} \sum_{k} C_{k} \left[ \frac{\dot{q}_{k}(0)}{s^{2} + \omega_{k}^{2}} + \frac{sq_{k}(0)}{s^{2} + \omega_{k}^{2}} \right] e^{st} ds , \end{aligned}$$

$$(7.4)$$

where the term on the right-hand side plays the role of an external force f(t) to the Brownian particle.

When we consider that  $\langle \dot{q}_k(0) \rangle = \langle q_k(0) \rangle = 0$  it is obvious that  $\langle f(t) \rangle = 0$ . Moreover, with the choice (1.10) for the spectral function  $J(\omega)$  and the use of the equipartition theorem we can show that  $\langle f(t)f(t') \rangle = 2\eta k_B T \delta(t-t')$ .

On the other hand, if we assume that the reservoir is in

thermal equilibrium with the particle at the position  $q_0$ , the fact that  $\langle f(t) \rangle = 0$  is no longer true. This is due to the form of (1.1) which can be rewritten as

$$L = \frac{1}{2}m\dot{q}^{2} - V(q) - \sum_{k} \frac{1}{2}\tilde{m}_{k}\omega_{k}^{2}(\tilde{q}_{k} - q)^{2} + \sum_{k} \frac{1}{2}\tilde{m}_{k}\tilde{q}_{k}^{2},$$
(7.5)

where

$$\widetilde{q}_k \equiv \frac{m_k \omega_k^2}{C_k} q_k, \quad \widetilde{m}_k \equiv \frac{C_k^2}{m_k \omega_k^4} . \tag{7.6}$$

Therefore, it is the Lagrangian of a set of oscillators with their equilibrium positions right at the position q of the particle subject to a potential V(q). Consequently  $\langle f(t) \rangle \propto \langle q_k(0) \rangle = q_0$  is now finite. This is a forcing term to (7.4) and will generate another contribution to the time evolution of q(t). As we can easily see, both  $\langle q(t) \rangle$  and  $\langle p(t) \rangle$  given by (6.9) and (6.13), respectively, have extra contributions depending on  $\langle q \rangle_0$ .

An important point is that these terms do not appear in the case of a free damped particle (V=0). In this case the system is translation invariant and there is no preferred origin to the position q(t). The initial condition is always expressed in terms of  $\langle \dot{q}_k(0) \rangle$  which implies in  $\langle f(t) \rangle = 0$ .

In order to remedy this situation it is necessary to modify our model (1.1) in such a way that the particle only feels its environment locally. In our present model the particle interacts with the same set of oscillators no matter what its position is. Actually, there are more realistic models for the environment where this local character naturally shows up.<sup>13</sup>

As far as this issue is concerned it is more advantageous to work with the factorizable initial condition since it assumes the bath in thermal equilibrium regardless of the position of the particle at t=0. Consequently,  $\langle f(t) \rangle = 0$ .

Notice that this qualitative analysis only applies to the classical limit. In order to rigorously study this effect one should carefully analyze Eqs. (6.9) and (6.13) in the limit of low and high temperatures.

Finally, we wish to call the attention of the reader to the fact that dealing with generalized initial conditions implies that for each problem there is a completely new propagation kernel J(x,y,t;x',y',0). In the case of factorizable initial conditions the only modification from one problem to the other was the external potential V(q). Although we have treated an exactly soluble model we believe that the techniques used herein can be applied to more complex models within suitable approximations.

*Note.* Soon after we finished this work, we became aware of Refs. 14 and 15, in which the authors address very similar problems.

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# APPENDIX A: EVALUATION OF I([x], [y], x', y')

Let us start by defining the new variables

$$\widetilde{x} \equiv u - U/2, \quad \widetilde{x}' \equiv u' - U/2$$
 (A1)

in such a way that

$$z(u) = z(\tilde{x} + U/2) = \overline{z}(\tilde{x}) ,$$
  

$$z(u') = z(\tilde{x}' + U/2) = \overline{z}(\tilde{x}') ,$$
  

$$f(u) = f(\tilde{x} + U/2) = \overline{f}(\tilde{x}) ,$$
  
(A2)

where  $\overline{z}$  and  $\overline{f}$  are now defined within (-U/2, U/2). Replacing  $\tilde{x} \rightarrow u$  and  $\tilde{x}' \rightarrow u'$  we can write  $S_{\text{eff}}$  as

$$S_{\text{eff}}[z] = \int_{-U/2}^{U/2} du \left[ \frac{\eta}{4\pi} \int_{-\infty}^{\infty} du' \frac{\left[\overline{z}(u) - \overline{z}(u')\right]^2}{(u - u')^2} + \overline{f}(u)\overline{z}(u) + \frac{M}{2} \dot{\overline{z}}(u)^2 + \frac{M}{2} \omega_0^2 \overline{z}(u)^2 \right], \quad (A3)$$

where the frequency integration in (3.6) has already been evaluated for the case in question  $[J(\omega)=\eta\omega$  and  $V(q)=M\omega_0^2q^2/2$ ]. The shifted function  $\overline{f}(u)$  is

$$\bar{f}(u) = \frac{-\eta}{\pi} \int_{0}^{\Omega} d\omega \, \omega \int_{0}^{t} dt' [x(t') - y(t')] \operatorname{cosech}(\omega U/2) \\ \times (i \, \cos\omega t' \cosh\omega u \\ + \sin\omega t' \sinh\omega u) .$$
(A4)

Expanding  $\overline{z}(u)$  and  $\overline{f}(u)$  in Fourier series we have

$$\overline{z}(u) = \sum_{n = -\infty}^{\infty} \overline{z}_n e^{-i\omega_n u}, \quad \overline{f}(u) = \sum_{n = -\infty}^{\infty} \overline{f}_n e^{-i\omega_n u}, \quad (A5)$$

with  $\omega_n \equiv 2n \pi/U$ . Notice that since  $\overline{z}(u) = \overline{z}^{R}(u)$ + $i\overline{z}^{I}(u)$  and  $\overline{f}(u) = \overline{f}^{R}(u) + i\overline{f}^{I}(u)$  the coefficients  $\overline{z}_n$ and  $\overline{f}_n$  can be decomposed as

$$\overline{z}_n = \overline{z}_n^R + i \overline{z}_n^I ,$$
  

$$\overline{f}_n = \overline{f}_n^R + i \overline{f}_n^I ,$$
(A6)

where  $\overline{z}_{n}^{R}$ ,  $\overline{z}_{n}^{I}$ ,  $\overline{f}_{n}^{R}$ , and  $\overline{f}_{n}^{I}$  are all complex.

Now, inserting expansions (A5) in (A3) and (A4) and evaluating the integrals on u we can write the effective action as

$$S_{\text{eff}}[z] = \frac{MU}{2} \sum_{n=-\infty}^{\infty} (\omega_n^2 + 2\gamma |\omega_n| + \omega_0^2) \overline{z}_n \overline{z}_{-n} + U \sum_{n=-\infty}^{\infty} \overline{f}_n \overline{z}_{-n} , \qquad (A7)$$

where  $\gamma \equiv \eta/2M$  and  $\overline{f}_0$  and  $\overline{f}_n$  can be obtained from (A4) and (A5) as

(A10)

$$\overline{f}_{n} = \frac{-\eta i}{U\pi} \int_{0}^{\Omega} d\omega \,\omega \int_{0}^{t} dt' [x(t') - y(t')] \frac{2(-1)^{n}}{(\omega^{2} + \omega_{n}^{2})} \times (\omega \cos\omega t' - \omega_{n} \sin\omega t') .$$
(A8)

Evaluating the frequency integration when n = 0 we get

$$\bar{f}_n = \frac{-2i\eta(-1)^n}{U\pi} \int_0^t dt' [x(t') - y(t')] \left[ \frac{\Omega^2}{\Omega^2 + \omega_n^2} \frac{\sin\Omega t'}{t'} - \int_0^\Omega d\omega \frac{2\omega_n^2 \omega \sin\omega t'}{t'(\omega^2 + \omega_n^2)^2} - \int_0^\Omega d\omega \,\omega_n \frac{\sin\omega t'}{(\omega^2 + \omega_n^2)} \right]$$

Since we are interested in the long-time behavior of the system we must take the limit  $\Omega \rightarrow \infty$  in all our expressions. In this way we have

$$\bar{f}_{0} = \frac{-2i\eta}{U} \int_{0}^{t} dt' [x(t') - y(t')] \delta(t')$$
$$= \frac{-i\eta}{U} [x(0) - y(0)], \qquad (A11)$$

and if  $n \neq 0$ ,

$$\bar{f}_{n} = (-1)^{n} \bar{f}_{0} + \frac{2i\eta(-1)^{n}}{U\pi} \int_{0}^{t} dt' [x(t') - y(t')] \\ \times \left[ \frac{\pi |\omega_{n}| e^{-|\omega_{n}|t'}}{2} + \frac{\pi \omega_{n} e^{-|\omega_{n}|t'}}{2} \right].$$
(A12)

$$\bar{f}_{0} = \frac{-2i\eta}{U} \int_{0}^{t} dt' [x(t') - y(t')] \frac{1}{\pi} \frac{\sin\Omega t'}{t'}$$
(A9)

while for  $n \neq 0$  we can integrate the first term within brackets by parts and rewrite (A8) as

Here we notice that for 
$$n < 0$$
  $\overline{f} = (-1)^n \overline{f}_n$ 

Here we notice that for n < 0,  $\overline{f}_n = (-1)^n \overline{f}_0$ . Due to the fact that  $z^R(u)$  and  $z^I(u)$  are real quantities we must have  $\overline{z}_n^{R*} = \overline{z}_{-n}^R$  and  $\overline{z}_n^{I*} = \overline{z}_{-n}^I$ . Therefore, we can write

$$\overline{z}_{n}^{R} = \frac{a_{n}^{R} + ib_{n}^{R}}{2}, \quad \overline{z}_{-n}^{R} = \frac{a_{n}^{R} - ib_{n}^{R}}{2},$$

$$\overline{z}_{n}^{I} = \frac{a_{n}^{I} + ib_{n}^{I}}{2}, \quad \overline{z}_{-n}^{I} = \frac{a_{n}^{I} - ib_{n}^{I}}{2},$$
(A13)

where  $a_n^R$ ,  $b_n^R$ ,  $a_n^I$ , and  $b_n^I \in \mathbb{R}$  and finally rewrite (A17) as

$$S_{\text{eff}} = S_{\text{eff}}^R + i S_{\text{eff}}^I$$

where

$$S_{\text{eff}}^{R} = \frac{MU}{8} A_{0} [(a_{0}^{R})^{2} - (a_{0}^{I})^{2}] - \frac{U\tilde{f}_{0}a_{0}^{I}}{2} + \frac{U}{2} \sum_{n=1}^{\infty} \tilde{f}_{n} (b_{n}^{R} - a_{n}^{I}) + \frac{MU}{4} \sum_{n=1}^{\infty} A_{n} [(a_{n}^{R})^{2} + (b_{n}^{R})^{2} - (a_{n}^{I})^{2} - (b_{n}^{I})^{2}] - \frac{U\tilde{f}_{0}}{2} \sum_{n=1}^{\infty} (-1)^{n} (b_{n}^{R} + a_{n}^{I}), \qquad (A14)$$

$$S_{\text{eff}}^{I} = \frac{MU}{4} A_{0} a_{0}^{R} a_{0}^{I} + \frac{U\tilde{f}_{0}a_{0}^{R}}{2} + \frac{U}{2} \sum_{n=1}^{\infty} \tilde{f}_{n} (a_{n}^{R} + b_{n}^{I}) + \frac{MU}{2} \sum_{n=1}^{\infty} A_{n} (a_{n}^{R} a_{n}^{I} + b_{n}^{R} b_{n}^{I}) + \frac{U\tilde{f}_{0}}{2} \sum_{n=1}^{\infty} (-1)^{n} (a_{n}^{R} - b_{n}^{I}), \qquad (A15)$$

with

$$A_n \equiv \omega_n^2 + 2\gamma |\omega_n| + \omega_0^2 , \qquad (A16)$$

$$\tilde{f}_n = -i\bar{f}_n \ . \tag{A17}$$

The boundary conditions  $z(0) = \overline{z}(-U/2) = y'$  and  $z(U) = \overline{z}(U/2) = x'$  can also be expressed in terms of  $a_n$ 's and  $b_n$ 's. In order to do this we first split the trajectory  $\overline{z}(u)$  in two parts: A symmetric part  $\overline{z}_s(u)$  defined as

$$\overline{z}_{s}(u) = \frac{\overline{z}(u) + \overline{z}(-u)}{2}$$
(A18)

such that

$$\overline{z}_{s}(-U/2) = \overline{z}_{s}(U/2) = \frac{x'+y'}{2} \equiv q'$$
, (A19)

and an antisymmetric part  $\overline{z}_a(u)$ , given by

$$\overline{z}_{a}(u) = \frac{\overline{z}(u) - \overline{z}(-u)}{2}$$
(A20)

with boundary conditions

$$\overline{z}_a(-U/2) = \frac{-\xi'}{2}, \ \overline{z}_a(U/2) = \frac{\xi'}{2},$$
 (A21)

where  $\xi' \equiv x' - y'$ . This last boundary condition can still be written as

$$\lim_{\epsilon \to 0} \overline{z} \left[ \frac{U - \epsilon}{2} \right] - \overline{z} \left[ \frac{-(U - \epsilon)}{2} \right] = \xi' , \qquad (A22)$$

showing that there is a jump in the antisymmetric part of  $\overline{z}(u)$  exactly at  $u = \pm U/2$ . We shall perform all our calculations with finite  $\epsilon$  and only at the end take the limit when  $\epsilon \rightarrow 0$ . In terms of  $a_n$ 's and  $b_n$ 's it turns out that (A19) and (A22) become

$$q' = \frac{a_0^R}{2} + \sum_{n=1}^{\infty} a_n^R (-1)^n , \qquad (A23a)$$

$$0 = \frac{a_0^I}{2} + \sum_{n=1}^{\infty} a_n^I (-1)^n , \qquad (A23b)$$

$$\xi' = -2 \sum_{n=1}^{\infty} b_n^{R} (-1)^n \sin(\omega_n \epsilon/2) , \qquad (A23c)$$

$$0 = -2\sum_{n=1}^{\infty} b_n^I (-1)^n \sin(\omega_n \epsilon/2) . \qquad (A23d)$$

The next step in our approach is to extremize either  $S_{\text{eff}}^R$  or  $S_{\text{eff}}^I$  in (A14) and (A15) subject to the constraints (A23). Then, using the method of Lagrange multipliers, one can show that the wanted values for the  $a_n$ 's and  $b_n$ 's are

$$a_n^R = \frac{2q' A_0 (-1)^n}{B A_n}$$
, (A24a)

$$a_0^R = \frac{2q'}{B} \quad , \tag{A24b}$$

$$a_n^{I} = \frac{2(-1)^n}{MBA_n} (\tilde{f}_0/2 + A_0 P) - \frac{\tilde{f}_n}{MA_n} , \qquad (A24c)$$

$$a_0^I = \frac{2}{MB} (P - \tilde{f}_0 V) ,$$
 (A24d)

$$b_n^R = \frac{(-1)^n \sin(\omega_n \epsilon/2)}{MQ(\epsilon) A_n} (4R(\epsilon) - 4\tilde{f}_0 T(\epsilon) - 2M\xi') + \frac{\tilde{f}_0(-1)^n}{MA_n} - \frac{\tilde{f}_n}{MA_n} , \qquad (A24e)$$

$$b_n^I = 0$$
, (A24f)

$$b_0^{\kappa} = 0 , \qquad (A24g)$$

$$b_0^1 = 0$$
, (A24h)

where

$$V \equiv \sum_{n=1}^{\infty} 1/A_n , \qquad (A25)$$

$$P \equiv \sum_{n=1}^{\infty} \frac{\tilde{f}_n (-1)^n}{A_n} , \qquad (A26)$$

$$B \equiv 2 A_0 V + 1$$
, (A27)

$$T(\epsilon) \equiv \sum_{n=1}^{\infty} \frac{\sin(\omega_n \epsilon/2)}{A_n} , \qquad (A28)$$

$$R(\epsilon) \equiv \sum_{n=1}^{\infty} \frac{\tilde{f}_n(-1)^n \sin(\omega_n \epsilon/2)}{A_n} , \qquad (A29)$$

$$Q(\epsilon) \equiv 4 \sum_{n=1}^{\infty} \frac{\sin^2(\omega_n \epsilon/2)}{A_n} .$$
 (A30)

Now, substituting expressions (A24) in (A14) and (A15) one gets

$$\bar{S}_{\text{eff}} = \frac{MU(\xi')^2}{4Q(\epsilon)} - \frac{UZ(\epsilon)\xi'}{Q(\epsilon)} + \frac{MU}{2\kappa} \left[ q' + \frac{i\bar{P}}{M} \right]^2 + iUq'\tilde{f}_0 + \frac{UZ(\epsilon)^2}{Q(\epsilon)} , \qquad (A31)$$

where

$$Z(\epsilon) \equiv R(\epsilon) - \tilde{f}_0 T(\epsilon)$$
  
=  $\frac{2\eta}{U} \int_0^t dt' [x(t') - y(t')] \frac{\omega_n e^{-\omega_n t'} \sin \omega_n \epsilon/2}{A_n}$ ,  
(A32)

$$\mathbf{x} \equiv \frac{B}{A_0} = \sum_{n=-\infty}^{\infty} 1/A_n , \qquad (A33)$$

$$\overline{P} \equiv \sum_{n=1}^{\infty} \frac{\overline{f}_n (-1)^n}{A_n} , \qquad (A34)$$

and

1

$$\tilde{f}_n \equiv \tilde{f}_n - (-1)^n \tilde{f}_0 . \tag{A35}$$

The last step to obtain the final value of  $\overline{S}_{\text{eff}}$  is to take the limit  $\epsilon \rightarrow 0$  in (A31). This is done exactly in the same way as in Appendix B of Ref. 8. It is not a hard matter to show that

$$Q(\epsilon) = \frac{U}{2} [\epsilon - Q_2 \epsilon^2 + O(\epsilon^3)]$$
(A36)

and

$$Z(\epsilon) = \frac{\eta}{U} [Z_1 \epsilon + O(\epsilon^3)], \qquad (A37)$$

where

$$Q_2 = \frac{1}{U} \sum_{n=1}^{\infty} \left[ 1 - \frac{\omega_n^2}{A_n} \right]$$
(A38)

and

$$Z_{1} = \int_{0}^{t} dt' [x(t') - y(t')] \frac{\omega_{n}^{2} e^{-\omega_{n} t'}}{A_{n}} .$$
 (A39)

Equations (A36) and (A37) allow us to take the limit  $\epsilon \rightarrow 0$  of (A31). In this limit, one can easily see that the last term on the right-hand side of the latter vanishes while the second one will give us a finite contribution. The problem is the first term of  $\overline{S}_{\rm eff}$  which diverges as  $\epsilon^{-1}$ .

As it was argued in Ref. 8 this is due to the steep parts of the path at the end of the interval (-U/2, U/2). But since this is a consequence of expanding a discontinuous function in terms of continuous ones we must not take this divergent contribution into account.

After taking the limit  $\epsilon \rightarrow 0$  we must convert all the sums over  $\omega_n$  into integrals (with the help of appropriate contour integrations) to finally get

3114

$$\overline{S}_{\text{eff}} = \frac{\eta}{2\pi} \int_{0}^{\Omega} d\omega \frac{\omega^{3} \coth(\omega U/2)}{(\omega_{0}^{2} - \omega^{2})^{2} + 4\gamma^{2} \omega^{2}} \left[ (\xi')^{2} - \xi' \int_{0}^{t} dt' \xi(t') \left[ \frac{2(\omega^{2} - \omega_{0}^{2})}{\omega} \sin\omega t' - \frac{2\eta}{M} \cos\omega t' \right] \right] \\ + \frac{MU}{2\kappa} \left[ q' + \frac{2i\gamma}{\pi} \int_{0}^{t} dt' \int_{0}^{\Omega} d\omega \frac{\omega \coth(\omega U/2)}{(\omega_{0}^{2} - \omega^{2})^{2} + 4\gamma^{2} \omega^{2}} \xi(t') \left[ (\omega_{0}^{2} - \omega^{2}) \cos\omega t' - \frac{\eta}{M} \omega \sin\omega t' \right] \right]^{2} - i\eta q' \xi' , \quad (A40)$$

where we have introduced new paths  $\xi(t')$  and q(t') as

$$\xi(t') \equiv x(t') - y(t'), \quad q(t') \equiv \frac{x(t') + y(t')}{2}$$

#### APPENDIX B: THE FUNCTION $I_0(t)$

As we know,  $tr\tilde{\rho} = 1$  or

$$\int \tilde{\rho}(q,0,t) dq = 1 . \tag{B1}$$

Then using (5.10) with  $\xi = 0$  and (1.4) we have

$$\widetilde{\rho}(q,0,t) = \int \int dq' d\xi' \widetilde{\rho}_0(q',\xi',0) J(q,0,t;q',\xi',0) .$$
 (B2)

Substituting (B2) in (B1), the integral over q can immediately be done yielding

$$\int dq J(q,0,t;q',\xi',0) \propto \frac{2\pi\hbar}{N(t)} \delta(\xi') .$$
(B3)

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Then, evaluating the integral over  $\xi'$  we get

$$\int dq' \exp\left[\frac{-(q')^2}{2\hbar\lambda}\right] \widetilde{\rho}_0(q',0,0) \frac{2\pi\hbar}{N(t)} I_0(t) = 1 . \quad (B4)$$

But since we know that [see (2.12)]

$$\int dq' \exp\left[\frac{-(q')^2}{2\hbar\lambda}\right] \widetilde{\rho}_0(q',0,0) = 1 , \qquad (B5)$$

one has

$$I_0(t) = \frac{N(t)}{2\pi\hbar} . \tag{B6}$$

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(A41)