Dissipative quantum dynamics in a boson bath

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We investigate the dynamics of a quantum particle coupled to a boson heat bath. Using a real-time path-integral formalism, we obtain the Wigner distribution of the particle in the form of a power series in the strength of the anharmonicity V_0. This series is shown to converge for all V_0 when t is fixed and for small V_0 uniformly in t. The latter proves the convergence to equilibrium for small anharmonicities. The effects of initial conditions on the evolution are studied by explicitly considering two types of initial states: product states and mixed Gibbs states. We show that in certain cases the evolution of the mixed states which avoid many pathologies of the product states, arising from the removal of the cutoff on the frequency distribution of the bath, can be related to that of product states when the latter are started at $t=-\infty$. We also solve exactly a simple stationary nonequilibrium model, a harmonic system in contact with two thermal baths, and derive an alternative criterion for a practically useful quasiclassical approximation. Finally, some connections to the Josephson junction are discussed. These include (a) the Green-Kubo-Einstein relation between the mobility and the diffusion constant of the washboard potential and (b) the time evolution of a rf superconducting quantum interference device.

I. INTRODUCTION

The dissipative dynamics of a quantum system, with one or few degrees of freedom, coupled to a heat-bath environment, has been the subject of many investigations: for a general review and references see Refs. 1–3. Given an initial state of the whole system, consisting of a particle plus the environment, we are interested in the evolution of the reduced density matrix of the particle obtained by tracing out of the bath degrees of freedom. In contrast to the classical case there are severe restrictions, physical and technical, on the type of initial states one can deal with for a quantum system.[4,5] There are also problems with the "approach to equilibrium;" only the free and harmonic cases have been studied carefully. In this paper, we investigate the time evolution of two kinds of initial states: the product state[1-3] and the mixed Gibbs state.[5] By using the Keldysh technique[6] (where one looks at the quantum time-ordered evolution along the complex Baym-Kadanoff contour[7]) the different initial states can be treated in the same framework and the trace over the environmental variables done in a compact form. This is carried out in Sec. II for a general frequency distribution of the bath and both types of initial states. It yields the Wigner distributions[8] of anharmonic systems in the form of a power series in the anharmonicity V_0.

In Sec. III we study the problem of approach to equilibrium in the Ohmic limit where the dissipation spectrum is linear at low frequencies. We also discuss there the relation between the two kinds of initial states and the problem of removing the cutoff of the frequency distribution of the heat bath. In Sec. IV, a nonequilibrium model consisting of two thermal baths and two harmonic oscillators is further considered. Section V is devoted to the quasiclassical approximation.[9] This approximation replaces the operator Langevin equation (which is difficult to solve) by a quasiclassical c-number version of it, taking, however, the spectrum of the random noise to be colored in a suitable way. We derive a criterion for the validity of this approximation by using the results of Sec. II. Finally, in Sec. VI we discuss two problems related to the Josephson junction: (1) the mobility, diffusion constant, and the Einstein relation associated with the current-biased junction; (2) the time evolution of the rf SQUID with a mixed initial state. Since the mobility in (1) has been extensively studied recently,[10-12] we mainly focus here on the discussion of the Einstein relation.

Some algebraic work is put in the appendixes. There are four of them: Appendix A contains the derivation of the path-integral formalism; Appendix B contains the basic mathematical work associated with the mixed initial state; Appendix C evaluates the Jacobian of the path integration over the center-of-mass paths in the presence of nonlocal (retarded) interactions; and finally, Appendix D gives the upper bound of the anharmonic expansion required in Sec. III B.

II. GENERAL FORMALISM

A. The reduced density matrix

We consider a system consisting of a particle of mass M moving in a potential $V(x)$ and a "heat bath" representing its environment. The total Hamiltonian is

$$\hat{H}=\hat{H}_p+\hat{H}_c+\hat{H}_e \;, \tag{2.1}$$

with

$$\hat{H}_p=\frac{\hat{p}^2}{2M}+V(\hat{x}) \;, \tag{2.2a}$$

$$\hat{H}_e=\sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k \;, \tag{2.2b}$$

the particle's and environment's Hamiltonian, and

$$\hat{H}_c=\hat{x}\sum_k C_k(\hat{a}_k^\dagger+\hat{a}_k)+\sum_k \frac{C_k^2}{\hbar\omega_k}\hat{x}^2 , \tag{2.2c}$$

the coupling interaction [the second term in (2.2c) cancels the adiabatic potential shift induced by the first term]. $\{\hat{a}_k,\hat{a}_k^\dagger\}$ is the set of creation and annihilation operators of the boson bath and the carets indicate that the objects are operators. It is convenient to introduce the dissipation spectrum[1-3] defined as

$$J(\omega)=\pi\sum_k C_k^2[\delta(\omega-\omega_k)-\delta(\omega+\omega_k)] , \tag{2.3}$$

which will be taken, in the thermodynamic limit, to be a smooth function of ω.

Given a density matrix $\hat{\mu}(0)$ at time 0, we call $\hat{\rho}(t)=\mathrm{Tr}_e[\hat{\mu}(t)]$ the reduced density matrix for the particle (where the subscript e indicates the "environment") and write its position representation in terms of the symmetric, $Q=(x+x')/2$, and antisymmetric, $r=(x-x')$, coordinates,

$$\rho(Q,r,t)\equiv\langle Q+r/2|\hat{\rho}(t)|Q-r/2\rangle . \tag{2.4}$$

The Wigner distribution[8] is then given by

$$w(Q,P,t)\equiv\int\frac{dr}{2\pi\hbar}\rho(Q,r,t)\exp\left[-\frac{i}{\hbar}Pr\right] . \tag{2.5}$$

We will consider the following two kinds of initial states: (A) A product state[1-3,13] given by

$$\hat{\mu}_P(0)=\hat{\rho}(0)\exp(-\beta\hat{H}_e)/\mathrm{Tr}_e[\exp(-\beta\hat{H}_e)] , \tag{2.6}$$

where $\hat{\rho}(0)$ operates on the particle's variables only. The product initial state, though somewhat artificial and beset with serious difficulties in certain limits,[4,5] is very convenient for computations. Physically, the product state assumes a sudden switch-on of the coupling at $t=0^+$. (B) An equilibrium type of state in which the particle and the bath are coupled as in (2.2b) and (2.2c),

$$\hat{\mu}_M(0)=\frac{\exp[-\beta(\hat{H}_e+\hat{H}_c+\hat{\hat{H}}_p)]}{\mathrm{Tr}\exp[-\beta(\hat{H}_e+\hat{H}_c+\hat{\hat{H}}_p)]} , \tag{2.7a}$$

where

$$\hat{\hat{H}}_p=\frac{\hat{p}^2}{2M}+V_i(\hat{x}) , \tag{2.7b}$$

with $V_i(\hat{x})$ an "initial potential" which can differ from $V(\hat{x})$ in (2.2a). The physical meaning of this "mixed initial" state is that the system is prepared by letting the particle equilibrate with the bath under the potential $V_i(\hat{x})$. If $V_i(\hat{x})=V(\hat{x})$, then the total system is in thermal equilibrium at $t=0$ and will remain so for all t. In practice it is often convenient to choose $V_i(\hat{x})$ to be a quadratic confining potential.[5]

The evolution of the reduced density matrix for a type-(A) initial state can be written as a linear transformation of the initial ρ:

$$\rho(Q_f,r_f,t)\equiv\int dQ_i dr_i J_P(Q_f,r_f,t;Q_i,r_i,0)\rho(Q_i,r_i,0) , \tag{2.8a}$$

where the subscripts f and i are to remind us of the final and initial values of the path. There is no corresponding transformation independent of $\rho(Q,r,0)$ for a type-(B) state. It is nevertheless convenient to write ρ at time t in the form

$$\rho(Q_f,r_f,t)\equiv\int dQ_i dr_i J_M(Q_f,r_f,t;Q_i,r_i,0)(Z_r)^{-1} , \tag{2.8b}$$

where

$$Z_r=\frac{\mathrm{Tr}\exp[-\beta(\hat{H}_e+\hat{H}_c+\hat{\hat{H}}_p)]}{\mathrm{Tr}_e(e^{-\beta\hat{H}_e})}$$

is just a constant. In this form both J_P and J_M can be expressed in terms of path integrals over a contour γ_α, see Fig. 1,

$$J_\alpha(Q_f,r_f,t;Q_i,r_i,0)\equiv\int_{\tau\in\gamma_\alpha}\mathcal{D}z(\tau)\exp\left[\frac{i}{\hbar}S_\alpha[z(\tau)]\right]F_\alpha[z(\tau)] , \tag{2.9}$$

where $\alpha=P$ or M corresponds to the two kinds of initial states; $S_\alpha[z(\tau)]$ is the bare action of the particle and $F_\alpha[z(\tau)]$, which contains all the influences from the heat bath, is given in (A8). The boundary conditions associated with (2.9) are also stated in Appendix A. In particular, for the product state the contour γ_P on which the

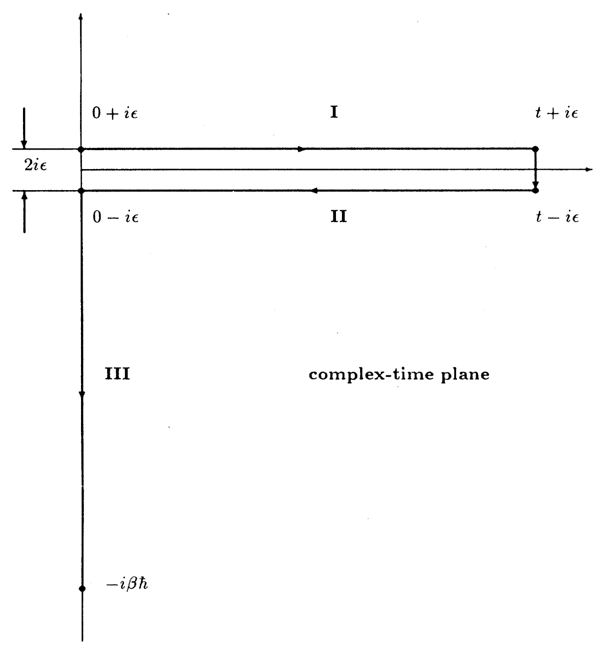

FIG. 1. Schematic representation of the (Baym-Kadanoff) contour γ. Note that the quantity ϵ is infinitesimal.

path integral is defined consists of only the first two parts of γ, $\gamma_{\rm I}$ and $\gamma_{\rm II}$, whereas for the mixed state $\gamma_M = \gamma$ with $V(z(\tau)) \equiv V_i(z(\tau))$ for $\tau \in \gamma_{\rm III}$. In the latter case one has to face the difficulties arising from the coupling between the real and imaginary axes.

B. The influence functional

It is convenient to introduce the center-of-mass and relative coordinates by

$$Q(\tau) \equiv \frac{z(\tau+i\epsilon)+z(\tau-i\epsilon)}{2} ,$$

$$r(\tau) = z(\tau+i\epsilon) - z(\tau-i\epsilon), \quad \tau \in [0,t]$$

and combine $\gamma_{\rm I}$ and $\gamma_{\rm II}$ (the forward and backward contours) into a single contour running from 0 to t. It is then easy to find for *the product initial state* the influence functional[1,13]

$$F_P[Q,r] \equiv \exp\left[-\frac{1}{\hbar^2}\int_0^t d\tau \int_0^\tau d\tau' r(\tau)\alpha_2(\tau-\tau')r(\tau') - \frac{i}{\hbar}\int_0^t d\tau \left[\int_0^\tau d\tau' r(\tau)\alpha_1(\tau-\tau')\dot{Q}(\tau') + r(\tau)\alpha_1(\tau)Q_i \right] \right] , \tag{2.10}$$

where

$$\alpha_1(\tau) = 2\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{J(\omega)}{\omega} \cos(\omega\tau) , \tag{2.11a}$$

$$\alpha_2(\tau) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} J(\omega)\hbar \coth\left[\frac{\beta\hbar\omega}{2}\right] \cos(\omega\tau) \tag{2.11b}$$

and $J(\omega)$ is defined in (2.3).

To obtain the influence functional for the mixed initial state we need to first carry out the additional path integral over the segment $\gamma_{\rm III}$, i.e., over the imaginary-time axis. Restricting ourselves to the case $V_i(\hat{x}) = M\omega_0 \hat{x}^2/2$ and denoting the integration variable by $q(\tau)$ with $\tau \in [0,\beta\hbar]$, we find

$$F_M[Q,r] = F_P[Q,r] I[Q,r] . \tag{2.12a}$$

$I[Q,r]$ is the path integral

$$I[Q,r] = \int_{q(0)=Q_i - r_i/2}^{q(\beta\hbar)=Q_i + r_i/2} \mathcal{D}q(\tau) \exp\{-S[q(\tau)]\} , \tag{2.12b}$$

where $S[q(\tau)]$ is the total effective imaginary time (Euclidean) action which contains also the influence from the real axis. To obtain it we define the Fourier transform

$$q(\tau) = \sum_{-\infty}^{\infty} q_n \exp(i\nu_n\tau), \quad \nu_n = \frac{2\pi n}{\beta\hbar}, \ n \text{ integer} . \tag{2.13a}$$

$S[q(\tau)]$ can then be written as

$$S[q(\tau)] = \frac{\beta}{2}\sum_{n=-\infty}^{\infty} K_n |q_n|^2 - i\sum_{-\infty}^{\infty} q_n f_n , \tag{2.13b}$$

with

$$K_n = M(\nu_n^2 + \omega_0^2) + 2\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{J(\omega)\nu_n^2}{\omega(\omega^2+\nu_n^2)} , \tag{2.13c}$$

$$f_n = \frac{2}{\hbar}\int_0^t ds\, r(s) \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{J(\omega)}{\omega^2+\nu_n^2} [\omega\cos(\omega s) + \nu_n \sin(\omega s)] \right] . \tag{2.13d}$$

This gives, see Appendix B,

$$I[Q,r] = Z_r \frac{1}{(2\pi\sigma_x)^{1/2}} \exp\left[-\frac{\sigma_p r_i^2}{2\hbar^2} - \frac{1}{2\sigma_x}\left[Q_i - i\sum_{n=-\infty}^{\infty} \frac{f_n}{\beta K_n} \right]^2 - \frac{1}{2}\sum_{n=-\infty}^{\infty} \frac{f_n f_{-n}}{\beta K_n} - \frac{r_i}{\hbar}\sum_{n=-\infty}^{\infty} \frac{M f_n \nu_n}{\beta K_n} \right] , \tag{2.14a}$$

where

$$\sigma_x = \sum_{n=-\infty}^{\infty} \frac{1}{\beta K_n}, \quad \sigma_p = \sum_{n=-\infty}^{\infty} \frac{M(K_n - M n_n^2)}{\beta K_n} \tag{2.14b}$$

are, respectively, the mean-square position and momentum of the particle in the potential $V_i(\hat{x})$. Note that the first factor Z_r on the right side of (2.14a) cancels exactly with that in (2.8b). In the Ohmic limit the various expressions can be evaluated more explicitly; they are presented in Appendix B.

C. Wigner distribution

In the rest of this section, we shall only consider type-(A) states; the corresponding results for the type-(B) states will be discussed in Secs. III and VI. Note that the first term in (2.10) can be expressed in terms of an average over a Gaussian stochastic process[14]

$$\exp\left[-\frac{1}{\hbar^2}\int_0^t d\tau \int_0^\tau d\tau' r(\tau)\alpha_2(\tau-\tau')r(\tau')\right]$$
$$\equiv\left\langle \exp\left[\frac{i}{\hbar}\int_0^t d\tau\, r(\tau)\xi(\tau)\right]\right\rangle_\xi , \quad (2.15a)$$

where $\xi(\tau)$ is Gaussian noise with covariance

$$\langle \xi(\tau)\xi(\tau')\rangle = \alpha_2(\tau-\tau') . \quad (2.15b)$$

We can now incorporate the influence function (2.10) into the bare action of the particle. This leads to

$$J_P(Q_f,r_f,t;Q_i,r_i,0)$$
$$=\left\langle \int \mathcal{D}Q\,\mathcal{D}r \exp\left[-\left[\frac{i}{\hbar}S_{\mathrm{eff}}[Q,r]\right]\right]\right\rangle_\xi \quad (2.16)$$

with

$$S_{\mathrm{eff}}[Q,r]$$
$$=\int_0^t d\tau \left[M\dot{r}\dot{Q}+V\left[Q-\frac{r}{2}\right]-V\left[Q+\frac{r}{2}\right] -r\left[\alpha_1(\tau)Q_i-\xi(\tau) +\int_0^\tau d\tau' \alpha_1(\tau-\tau')\dot{Q}(\tau')\right]\right] . \quad (2.17)$$

We next decompose the potential into two parts,

$$V(x)=V_h(x)+V_a(x) \quad (2.18)$$

with

$$V_h(x)=\tfrac{1}{2}M\omega_0^2x^2-Fx \quad (2.19a)$$

and $V_a(x)$ is an anharmonic potential which we choose for concreteness to have the form[10–12]

$$V_a(\hat{x})=V_0\cos[k_0(\hat{x}-b)] . \quad (2.19b)$$

1. Harmonic case

When $V_a(x)=0$ we can easily integrate over $r(\tau)$. Evaluating the path integral in a standard way,[15] namely discretizing time by steps $\epsilon=t/N$, we find that it gives a δ function over the path space of $Q(\tau)$ (we keep track of the exact prefactor of the path integral):

$$\frac{1}{2\pi\hbar}\left[\frac{M}{\epsilon}\right]^N \prod_{k=1}^{N-1}\delta(Y_k) , \quad (2.20a)$$

where

$$Y_k=-M\frac{Q_{k+1}-2Q_k+Q_{k-1}}{\epsilon}-\epsilon V_h'(Q_k)+\epsilon\xi_k -\epsilon\sum_{m=1}^{k}(Q_m-Q_{m-1})\alpha_1(k\epsilon-m\epsilon)-\epsilon Q_i\alpha_1(k\epsilon) . \quad (2.20b)$$

The δ functions indicate that the paths $Q(\tau)$ are restricted to the solutions of the generalized Langevin equation with memory

$$M\ddot{Q}+\int_0^\tau d\tau\,\alpha_1(\tau-\tau')\dot{Q}(\tau')+V_h'(Q)=\xi(\tau)-\alpha_1(\tau)Q_i . \quad (2.21)$$

To integrate over $Q(\tau)$, we need to find both the solution(s) of the Langevin equation (2.21) with the fixed boundary condition $Q(0)=Q_i$, $Q(t)=Q_f$, and the Jacobian of the transformation (2.20b). The latter is calculated explicitly in Appendix C *for a general potential and arbitrary dissipation spectrum* $J(\omega)$. For the harmonic potential, the transformation (2.20b) is linear so that the Jacobian is path independent and can therefore be determined from the normalization of the final density matrix. This gives

$$J_P(Q_f,r_f,t;Q_i,r_i,0)=\left\langle \left[\left[\frac{2\pi\hbar}{M}\right]\left|\frac{\partial Q_f}{\partial \dot{Q}_i}\right|\right]^{-1}\exp\left[\frac{i}{\hbar}(M\dot{Q}_f r_f - M\dot{Q}_i r_i)\right]\right\rangle_\xi , \quad (2.22)$$

where $\dot{Q}_i$ and $\dot{Q}_f$ are the initial and final velocities determined from the solution of the Langevin equation (2.21). It should be emphasized that the boundary phases in (2.22), which are often ignored or incorrectly presented in the literature, are very important to ensure correct final results. In general there may exist, for a given t and (Q_f,Q_i), a number of $(\dot{Q}_f,\dot{Q}_i)$ that satisfy Eq. (2.21). It is therefore convenient to transform the fixed boundary problem into an initial-value problem. Hence, rather than fixing (Q_i,Q_f), we start with a given $(Q_i,\dot{Q}_i)$ and obtain the solution $(Q(t),\dot{Q}(t))$ at the final time. Then, using (2.22), it is not difficult to find

$$J_P(Q_f,r_f,t;Q_i,r_i,0)=\left\langle \frac{M}{2\pi\hbar}\int d\dot{Q}_i\,\delta(Q_f-Q(t))\exp\left[\frac{i}{\hbar}M[\dot{Q}(t)r_f-\dot{Q}_i r_i]\right]\right\rangle_\xi . \quad (2.23)$$

This gives the Wigner distribution

$$w(Q_f,P_f,t)=\left\langle \int dQ_i dP_i\, w(Q_i,P_i,0)\delta(Q_f-Q(t))\delta(P_f-P(t))\right\rangle_\xi = \langle \delta(Q_f-Q(t))\delta(P_f-P(t))\rangle , \quad (2.24)$$

where $P(t)=M\dot{Q}(t)$, $P_i=M\dot{Q}_i$, and the average $\langle\ \rangle$ without the subscript ξ is now with respect to both the initial distribution and the Gaussian random process. If the initial distribution is also Gaussian, as is often the choice in practice, we can use

$$\delta(x)=\int_{-\infty}^{\infty}\frac{dy}{2\pi}\exp(ixy)$$

and bring the average up to the exponent. It is then simple to find the final distribution,

$$w(Q_f,P_f,t)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}dy\,dy'\exp\left[-\frac{\langle\{y[Q_f-Q(t)]+y'[P_f-P(t)]\}^2\rangle}{2}\right]. \tag{2.25}$$

2. Anharmonic case

Following Fisher and Zwerger,[10] we expand the exponential of the effective action (2.17) via

$$\exp\left[-\frac{i}{\hbar}\int_0^t d\tau[V_1(Q+r/2)-V_a(Q-r/2)]\right]$$
$$\equiv 1+\sum_{n=1}^{\infty}\left[\left[\frac{V_0}{\hbar}\right]^n\int_0^t dt_n\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1K_n(t_n,t_{n-1},\ldots,t_1)\right], \tag{2.26a}$$

where

$$K_n(t_n,t_{n-1},\ldots,t_1)=\sum_{\{\sigma_j=\pm1\}}\left[\left[\prod_{j=1}^{n}\sigma_j\sin\{k_0[Q(t_j)-b]\}\right]\exp\left[\frac{i}{\hbar}\int_0^t d\tau\frac{\hbar k_0 r(\tau)}{2}\sum_{j=1}^{n}\sigma_j\delta(\tau-t_j)\right]\right]. \tag{2.26b}$$

Each order contributes to the remaining action (being quadratic or linear) a term linear in $r(\tau)$; this new term represents a series of δ forces. Therefore, we can carry out exactly the path integrations as before once we solve the modified Langevin equation in the presence of the δ forces [cf. (2.21)]:

$$M\ddot{Q}+\int_0^\tau d\tau'\alpha_1(\tau-\tau')\dot{Q}(\tau')+V_h'(Q)=\alpha_1(\tau)Q_i+\frac{k_0}{2}\sum_{j=1}^{n}\sigma_j\delta(\tau-t_j)+\xi(\tau). \tag{2.27}$$

The solution of (2.27) can be decomposed into two parts

$$Q_n(Q_i,P_i,\tau{:}[\xi(\tau')])=Q_0(Q_i,P_i,\tau{:}[\xi(\tau')])+\frac{k_0}{2}\sum_{j=1}^{n}\sigma_j g(\tau-t_j), \tag{2.28}$$

where Q_0 is the solution in the absence of the δ forces and is subject to the initial condition $Q_0(0)=Q_i$, $P(0)=P_i$, $g(\tau)$ is the Green's function of the homogeneous part,

$$M\ddot{g}(\tau)+\int_0^\tau d\tau'\alpha_1(\tau-\tau')\dot{g}(\tau')+M\omega_0^2 g(\tau)=\delta(\tau) \tag{2.29a}$$

with the initial condition

$$g(\tau)=\dot{g}(\tau)=0 \quad\text{for } \tau<0. \tag{2.29b}$$

The Wigner distribution at time t is now given by

$$w(Q_f,P_f,t)=\Bigg\langle\delta(Q_f-Q_0(t))\delta(P_f-P_0(t))+\sum_{n=1}^{\infty}\left[\left[\frac{V_0}{\hbar}\right]^n\int_0^t dt_n\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\sum_{\{\sigma_j=\pm1\}}\delta(Q_f-Q_n(t))\delta(P_f-P_n(t))\right.$$
$$\left.\times\prod_{j=1}^{n}\sigma_j\sin\{k_0[Q_n(t_j)-b]\}\right]\Bigg\rangle, \tag{2.30}$$

where the average is again with respect to both the initial distribution and the Gaussian random process. Note that (2.30) is formally exact. Thus given a function $A(\hat{x},\hat{p})$ its expectation value at time t is[8]

$$\langle A\rangle=\int dQ_f dP_f w(Q_f,P_f,t)A_w(Q_f,P_f)=\sum_{n=0}^{\infty}C_n(t)V_0^n, \tag{2.31}$$

where $A_w(Q,P)$ is the Wigner representation of $A(\hat{x},\hat{p})$,

$$A_w(Q,P)=\int_{-\infty}^{\infty} dr\langle Q+r/2|A(\hat{x},\hat{p})|Q-r/2\rangle \times\exp\left[-iP\frac{r}{\hbar}\right] . \quad (2.32)$$

The right side of (2.31) will converge absolutely for finite t provided the integrands involving A_w are bounded in absolute value—a condition usually satisfied for physically interesting quantities.

Equation (2.30) gives, in principle, the exact solution of the dynamics in the cosine potential; the generalization to the case involving many cosine potentials is evident. *The corresponding formula for the type-(B) states is discussed in Secs. III B and VI B.* Equations (2.30) and (2.31) are used to investigate the approach to equilibrium in the next section and the quasiclassical approximation in Sec. V.

III. CUTOFF, APPROACH TO EQUILIBRIUM, AND THE MIXED INITIAL STATE

We now study the limit where the number of degrees of freedom of the environment tends to infinity in such a way that the spectrum (2.3) can be replaced by a smooth function. Moreover, we consider the case where the spectrum $J(\omega)$ is linear in ω for small frequencies (Ohmic damping) and goes to zero at high frequencies, $\omega \gg \omega_c$, ω_c,

$$J(\omega)=\eta\omega f(\omega/\omega_c) ;$$
$$f(x)\to 1 \text{ for } x\to 0, \quad f(x)\to 0 \text{ for } x\to\infty . \quad (3.1)$$

η will be identified as the viscosity of the particle in the classical limit. For concreteness in this paper we shall choose the so-called "Lorentzian cutoff,"

$$f(x)=\frac{1}{1+x^2} . \quad (3.2)$$

A. Approach to equilibrium for anharmonic potential

Let us first briefly mention the harmonic case, which has been widely studied in the literature.[5,16,17] From the Langevin equation (2.21) and the Wigner distribution (2.24), one immediately sees that when $J(\omega)$ is given by (3.1) and (3.2) the system will always approach equilibrium (independent of the cutoff). For a general spectrum $J(\omega)$, the sufficient condition for approach to equilibrium can be stated in terms of an elegant inequality, see Ref. 17,

$$\left|\int_0^{\infty} d\omega \ln[J(\omega)]/(1+\omega^2)\right| < \infty .$$

It is straightforward to find that the final Wigner distribution, agreeing with the imaginary-time result, reads simply

$$\lim_{t\to\infty} w(Q,P,t)=(2\pi\sqrt{\sigma_x\sigma_p})^{-1}\exp\left[-\frac{Q^2}{2\sigma_x}-\frac{P^2}{2\sigma_p}\right] , \quad (3.3)$$

where σ_x and σ_p are given in (B13). Note that σ_p *will diverge if the cutoff is removed.* This is the typical problem associated with the Ohmic damping, see Refs. 4 and 5: we shall return to this point later.

At first sight it seems that the analysis used for the harmonic potential should also be applicable to the anharmonic case discussed at the end of Sec. II. Consider for example the average final position of the particle (other quantities can be treated similarly). Then, using (2.31), we can rewrite the nth-order integrand in the form

$$\text{const}\times g(t-t_n)\sum_{\{\mu_j=\pm 1\}}\left[\prod_{k=1}^{n-1}\sin\left[\frac{\hbar}{2}k_0^2\sum_{j=k+1}^{n}\mu_j g(t_j-t_k)\right]\right]\exp\left[i\sum_{j=1}^{n}\mu_j\left[\frac{\pi}{2}+k_0[Q_0(t_j)-b)]\right]\right] , \quad (3.4)$$

where we have used

$$\sin\{k_0[Q_m(t_j)-b]\}=-\tfrac{1}{2}\sum_{\mu_j=\pm 1}\exp\left[i\mu_j\left[\frac{\pi}{2}+k_0[Q_n(t_j)-b]\right]\right] \quad (3.5)$$

and summed over all the σ_j's. Thus, the dependence on the initial distribution [through $Q_0(t)$, the pure harmonic solution just discussed] will decay in every order after a sufficiently long time (which depends on n) and the integrals over time will converge [because all the t_j's in (3.4) then have to be close to t] provided the condition for approach to equilibrium for the harmonic part is satisfied. This does not, however, guarantee that the infinite sum will behave in the same way; we can only be sure of this if the series converges uniformly with respect to t. In Appendix D, we show explicitly that *there exists a V_0, call it $\overline{V}$, such that for $V_0<\overline{V}$ it does behave so.* Hence, in this case we can take the limit $t\to\infty$ term by term to get the final result. This implies in particular that for $V_0<\overline{V}$ the final distribution is independent of the initial one.

Let us now compare the $t\to\infty$ result with that calculated from the equilibrium formula

$$\langle Q\rangle\equiv\frac{\text{Tr}[\hat{x}\exp(-\beta\hat{H})]}{\text{Tr}[\exp(-\beta\hat{H})]} . \quad (3.6)$$

It is convenient to first trace out of the environmental degrees of freedom to obtain the reduced partition function (with a λ "source" for later use)

$$Z_r(\lambda)=\int_{q(0)=q(\beta\hbar)}\mathcal{D}q(\tau)\exp\left[\lambda q(0)-S_h[q(\tau)]-\int_0^{\beta\hbar}d\tau\frac{V_0}{\hbar}\cos\frac{2\pi}{q_0}[q(\tau)-b]\right], \tag{3.7}$$

where $S_h[q(\tau)]$ is the harmonic part of the Euclidean action defined by (2.13b) with $f_n=0$. In terms of this, (3.6) becomes

$$\langle Q\rangle=\left[\frac{d}{d\lambda}\ln Z_r(\lambda)\right]_{\lambda=0}. \tag{3.8}$$

We can now expand the partition function in terms of V_0 as in the real-time case,

$$Z_r(\lambda)=Z_0(\lambda)\sum_{n=0}^{\infty}\left[\frac{1}{n!}\left[\frac{-V_0}{2\hbar}\right]^n\int_0^{\beta\hbar}d\tau_n\cdots\int_0^{\beta\hbar}d\tau_1\sum_{\{\sigma_j=\pm1\}}\exp\left[ik_0\sum_{j=1}^{n}[\lambda W(\tau_j)-b]\sigma_j-\frac{k_0^2}{2}\sum_{j,j'=1}^{n}W(\tau-\tau')\sigma_j\sigma_{j'}\right]\right], \tag{3.9}$$

where Z_0 is the reduced partition function of the background harmonic part and $W(\tau)$ is its covariance

$$W(\tau)=\langle q(0)q(\tau)\rangle_0\,, \tag{3.10}$$

whose detailed expression is given in (B8). Clearly from (3.9) both the numerator and denominator in (3.6) are entire functions of V_0 (for fixed β). Furthermore the denominator does not vanish at $V_0=0$. Hence the expansion for $\langle Q\rangle$ in terms of V_0 must converge in the vicinity of $V_0=0$.

We now observe that the system must approach equilibrium at least within the common radius of convergence of both the "real-time" and "imaginary-time" expansions since (1) the final distribution at $t\to\infty$ is for $V_0<\bar{V}$ unique and independent of the initial state and (2) given an initial state corresponding to the equilibrium distribution of the whole system (particle plus environment) it will remain so at all time t. Note that (1) is valid only when the spectrum is continuous (which is possible only when the number of degrees of freedom of the environment is infinite), whereas (2) is always true.

B. The cutoff and the mixed initial states

There is a serious difficulty with the product initial state which has been noticed in Refs. 4 and 5. Taking the harmonic case as an example, the mean-square fluctuation of the coordinate of the particle obtained from the Langevin equation (2.21) has a divergent part (for $t>0$) when $\omega_c\to\infty$. For fixed ω_c, on the other hand, it decays exponentially to its equilibrium values as $t\to\infty$ whose coordinate part is well behaved as $\omega_c\to\infty$. (The mean-square fluctuation of the momentum is always divergent. This is unfortunately an intrinsic property of the ohmic damping but is of less importance.) The physical reason for this is that the product state assumes a sudden switch-on of the interaction between the particle and the bath.[5] This can become very severe if one is interested in macroscopic quantum coherence, macroscopic quantum tunneling, or related problems,[1-3] since the artificial switch-on of the coupling would very seriously influence the subsequent short-time behavior of the particle. A physically reasonable solution of this difficulty is to replace the product state by an appropriate mixed state.

The complications produced by using a mixed initial state are simplified somewhat if the initial potential $V_i(\hat{x})$ is quadratic. As is demonstrated in Appendix B, the mixed state can be replaced by a product state by putting the initial time of the latter at negative infinity and switching the potential form $V_i(\hat{x})$ to $V(\hat{x})$ at $t=0$. The algebra is rather lengthy but straightforward and the answer is rather evident: It works whenever the condition of approach to equilibrium is satisfied [for the potential $V_i(\hat{x})$]. In such a case the particle, starting at $t=-\infty$ in a product state, will equilibrate with the bath at $t=0$. Consequently the undesired divergences discussed above disappear since the switch-on is now put at $t=-\infty$. The equivalence simplifies the computations of various physical quantities for the mixed initial state (see Sec. VI). We expect that this kind of equivalence of the two kinds of initial states can be generalized to non-Ohmic damping and nonquadratic $V_i(\hat{x})$, e.g., for the cosine potential. Moreover, if the system of interest has several degrees of freedom, only those degrees directly coupled to the heat bath(s) will have divergent kinetic energies. This point is, among other things, explicitly demonstrated in the next section.

IV. NONEQUILIBRIUM STATIONARY STATE

We now consider a very simple nonequilibrium model, two interacting harmonic oscillators each coupled to its own heat bath. The two baths have different temperatures and different viscosities so that as $t\to\infty$ there will be a nonequilibrium stationary state. This model has been studied in detail in the classical regime where the stationary state is a Gaussian measure in which there are couplings between the position and momentum variables.[18] We wish to see what happens in the quantum regime where, as we have seen before, the momentum variables have a singular behavior. The extension of this model to the case where there is whole chain of oscillators between the two which are coupled to the heat baths can be done as in the classical case.[18]

The total Hamiltonian can be written as

$$\hat{H}=\frac{1}{2}\left[\frac{\hat{p}_1^2}{M_1}+M_1\omega_1^2\hat{x}_1^2\right]+\frac{1}{2}\left[\frac{\hat{p}_2^2}{M_2}+M_2\omega_2^2\hat{x}_2^2\right]+\frac{k}{2}(\hat{x}_1-\hat{x}_2)^2+\hat{H}_{c1}+\hat{H}_{c2}+\hat{H}_{e1}+\hat{H}_{e2}\ , \tag{4.1}$$

where we shall assume that the couplings and the Hamiltonians of the heat baths are the same as before, see (2.1) and (2.2). Taking the product initial state in which both baths are decoupled from the oscillators, we can trivially generalize our previous results for the evolution of the Wigner distribution to this situation,

$$w(\mathbf{Q}_f,\mathbf{P}_f,t)=\langle\delta(\mathbf{P}_f-\mathbf{P}(t))\delta(\mathbf{Q}_f-\mathbf{Q}(t))\rangle\ , \tag{4.2}$$

where we have used the vector notation $\mathbf{Q}$ for (Q_1,Q_2) and likewise for the momentum. Recall that the average $\langle\ \rangle$ is with respect to both the two random noises and the initial distribution $w(\mathbf{Q}_i,\mathbf{P}_i,0)$. For simplicity we shall, from now on, take the limit $\omega_c\to\infty$, which as explained before affects only the kinetic energy of the particles. The "equations of motion" for $\mathbf{Q}(\tau)$ are

$$M_1\ddot{Q}_1+\eta_1\dot{Q}_1+M_1\omega_1^2Q_1+k(Q_1-Q_2)=\xi_1(\tau)+\eta_1\delta(\tau)\ , \tag{4.3a}$$

$$M_2\ddot{Q}_2+\eta_2\dot{Q}_2+M_2\omega_2^2Q_2+k(Q_2-Q_1)=\xi_2(\tau)+\eta_2\delta(\tau)\ . \tag{4.3b}$$

Equations (4.3) are coupled linear equations whose solutions can be expressed as linear combinations of their eigenmodes. Note that these eigenmodes will be damped in time provided η_1 and/or η_2 is nonzero (simply due to energy conservation). Therefore for $t\to\infty$, the initial states will be forgotten and thus we need to consider only the final states.

To find the distribution at $t\to\infty$, it is most convenient to use the Fourier transform

$$\mathbf{Q}_F(\omega)=\int_{-\infty}^{\infty}\mathbf{Q}(t)e^{i\omega t}\ . \tag{4.4}$$

Then (4.3) take the form

$$[P_1(\omega)+k]Q_{1F}(\omega)-kQ_{2F}(\omega)=\xi_{1F}(\omega)\ , \tag{4.5a}$$

$$[P_2(\omega)+k]Q_{2F}(\omega)-kQ_{1F}(\omega)=\xi_{2F}(\omega)\ , \tag{4.5b}$$

where

$$P_j(\omega)\equiv M_j(\omega_j^2-\omega^2)-i\eta_j\omega,\quad j=1,2\ . \tag{4.6}$$

Equations (4.5) have the solution

$$Q_{1(2)F}(\omega)=\frac{P_{2(1)}(\omega)\xi_{1(2)}F^{(\omega)}+k[\xi_{1F}(\omega)+\xi_{2F}(\omega)]}{P_1(\omega)P_2(\omega)+k[P_1(\omega)+P_2(\omega)]}\ . \tag{4.7}$$

Note that the covariance of the Fourier transform of the noise is [cf. (2.11b) and (2.15)]

$$\langle\xi_{1(2)F}(\omega)\xi_{1(2)F}(\omega')\rangle=2\pi\delta(\omega+\omega')\eta_{1(2)}\hbar\omega\coth(\beta_{1(2)}\omega\hbar/2)\ , \tag{4.8a}$$

$$\langle\xi_{1F}(\omega)\xi_{2F}(\omega')\rangle=0\ . \tag{4.8b}$$

Given (4.7) and (4.8), it is not difficult to find the distribution at $t\to\infty$ via (3.17). The result is that the stationary measure is Gaussian with the covariances of the momenta being infinite while that of the coordinates is finite (but messy). The cross covariances are related to the energy flow which we discuss next.

Denoting the energy of subsystem 1 (2) consisting of the first (second) particle and the first (second) heat bath by

$$\hat{H}_j=\hat{H}_{pj}+\hat{H}_{cj}+\hat{H}_{ej},\quad j=1,2 \tag{4.9}$$

we have

$$\frac{d\hat{H}_1}{dt}=-\frac{k}{2M_1}[(\hat{x}_1-\hat{x}_2)\hat{p}_1+\hat{p}_1(\hat{x}_1-\hat{x}_2)]\ . \tag{4.10}$$

Since the total energy is conserved we can define the flux from subsystem 1 as

$$\hat{J}=\left[\frac{d\hat{H}_1}{dt}-\frac{d\hat{H}_2}{dt}\right]\Big/2 \tag{4.11}$$

and the average over the ensemble reads

$$\begin{aligned}J(t)&\equiv\mathrm{Tr}[\hat{J}\hat{\rho}(t)]\\&=-\frac{k}{2}\int d\mathbf{Q}_f d\mathbf{P}_f(Q_{1-f}-Q_{2f})\left[\frac{P_{1f}}{M_1}+\frac{P_{2f}}{M_2}\right]w(\mathbf{Q}_f,\mathbf{P}_f,t)\\&=-\frac{k}{2}\langle[Q_1(t)-Q_2(t)][\dot{Q}_1(t)+\dot{Q}_2(t)]\rangle\ .\end{aligned} \tag{4.12}$$

It is now straightforward to find the stationary flux

$$\lim_{t\to\infty}J(t)=k^2\eta_1\eta_2\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\omega^3\hbar[\coth(\beta_2\omega\hbar/2)-\coth(\beta_1\omega\hbar/2)]}{|P_1P_2+k(P_1+P_2)|^2}\ , \tag{4.13}$$

where the integral over the frequency is convergent. In the classical limit, $\hbar \to 0$, (4.13) reduces to the result of Casher and Lebowitz.[18] It is clear that in the quantum regime the flux is no longer proportional to the difference between the two temperatures; complicated quantum corrections arise when $\beta\hbar\omega \sim 1$, and in general we have to compute the flux numerically.

It is found from this two-particle case [see (4.7) and (4.8)] that only the particle(s) directly coupled to the heat bath(s) will be subject to the divergence of the momentum square disussed above. Thus, for a many-particle system, such as a harmonic chain, in contact with two baths at the ends [as considered in (Ref. 18)], the momentum distribution of the particle not in contact with the baths is well behaved for $\omega_c \to \infty$.

V. THE QUASICLASSICAL APPROXIMATION AND ITS JUSTIFICATION

In this section we discuss a quasiclassical approximation first proposed by Koch, VanHarlingen, and Clarke[9] in the context of Josephson junctions and further developed by Schmid[14] in the framework of path integrals. Going back to the effective action (2.15), we can expand

$$V(Q+r/2)-V(Q-r/2)=V'(Q)r+\frac{r^2}{24}V'''(Q)+\cdots \tag{5.1}$$

in a Taylor series. In regimes where the higher orders in (5.1) can be ignored, the path integral (2.16) becomes approximately

$$J_P(Q_f,r_f,t;Q_i,r_i,0)=\int \mathcal{D}Q\,\mathcal{D}r\,\exp\left\{\frac{i}{\hbar}\int_0^t d\tau\left[-V'(Q)r+\xi(\tau)r+M\dot{r}\dot{Q}-r\left[\alpha_1(\tau)+\int_0^\tau d\tau'\alpha_1(\tau-\tau')\dot{Q}(\tau')\right]\right]\right\}. \tag{5.2}$$

This can be evaluated in the same way as for the harmonic potential (see Sec. III C, except that the evaluation of the Jacobian of the path integral becomes nontrivial), leading to a Wigner distribution formally identical to (2.24) with $V_h(x)$ being replaced by the full potential $V(x)$. The result is the so-called quasiclassical approximation where the evolution of the particle is described by a c-number Langevin equation [see (2.21)] in which the noise spectrum is "colored."

To justify the approximation, Schmid[15] noted that the imaginary part of the effective action (2.15) acts to suppress fluctuations in $r(\tau)$. If the suppression is heavy, i.e., the viscosity is large (taking the Ohmic damping for example), then large fluctuations in $r(\tau)$ can be ignored. To get a more quantitative estimate, let us introduce a typical length scale L_0 for the anharmonicity. The validity of the quasiclassical approximation requires that for $r(\tau)\geq L_0$, the magnitude of the imaginary part of the action be much larger than 1, i.e.,

$$\frac{\eta L_0^2}{\pi\hbar} \gg 1\ , \tag{5.3}$$

see the appendix of Chen, Fisher, and Leggett[9] for further details.

To get a more precise criterion, consider the exact expression (2.30) and rewrite the path integral (5.2) (which is equivalent to the quasiclassical approximation) using the following identity [see (2.18) and (2.19) for $V_a(Q)$ and $V_h(Q)$]:

$$\int \mathcal{D}Q\,\mathcal{D}r\,\exp\left[\frac{i}{\hbar}\int_0^t d\tau[-V'(Q)r+\xi(\tau)r+\cdots]\right]$$
$$\equiv \int \mathcal{D}Q\,\exp\left[-\int_0^t d\tau\,V_a'(Q)\frac{\delta}{\delta\xi(\tau)}\right]\left[\int \mathcal{D}r\,\exp\left[\frac{i}{\hbar}\int_0^t d\tau[-V_h'(Q)r+(F+\xi)r+\ldots]\right]\right], \tag{5.4}$$

which can be easily verified by expanding the exponential (functional differential) operator into a power series. Substituting (5.4) into (5.2) we then can carry out the path integrations over $r(\tau)$ and $Q(\tau)$ as in Sec. II C. After some manipulations, we obtain an alternative expression for the Wigner distribution given in (2.24)

$$w(Q_f,P_f,t)=\left\langle \exp\left[-\int_0^t d\tau\,V_a'(Q_0(\tau))\frac{\overleftrightarrow{\delta}}{\delta\xi(\tau)}\right]\times\delta(Q_f-Q_0(t))\delta(P_f-P_0(t))\right\rangle, \tag{5.5}$$

which treats the anharmonic potential as a perturbation of the background harmonic potential $V_h(Q)$. The symbol $\overleftrightarrow{\delta}/\delta\xi$ indicates that each differential operates both to its right and left. A simple way to obtain (5.5) from (5.4) is to first do integration by parts so that the functional differentials act only on the measure of the noise (which is Gaussian). One then restores the differentials in the final stage by again integrating by parts.

We now consider how (5.5) can be obtained as an approximation to the exact expression (2.30) for the Wigner distribution. In that expression the quantity $k_0Q_n(\tau)$ is given by [see (2.21) and (2.29)]

$$k_0 Q_n(\tau) = \frac{\hbar k_0^2}{2} \sum_{j=1}^{n} \sigma_j g(\tau - t_j) + k_0 Q_0(\tau) \qquad (5.6)$$

so that if the first term on the right side is small, i.e.,

$$\frac{\hbar k_0^2 g_{\max}}{2} \ll 1 , \qquad (5.7)$$

where $g_{\max}$ is the maximum value of $g(\tau)$, we can treat it as a small perturbation. Then using [see (2.21) and (2.29)] the relation

$$\frac{\delta Q_0(\tau)}{\delta \xi(t_j)} \equiv g(\tau - t_j) \qquad (5.8)$$

the sum over $\{\sigma_j\}$ in (2.30) can be treated, to first order of $\hbar k_0^2 g_{\max}/2$, as taking derivatives, i.e., we can substitute

$$\sum_{\sigma_j = \pm 1} \sigma_j \to \hbar k_0 \frac{\delta}{\delta \xi(t_j)} \quad \text{and} \quad Q_n(\tau) \to Q_0(\tau) . \qquad (5.9)$$

To see this consider the following case:

$$\begin{aligned} \sum_{\sigma_j = \pm 1} \sigma_j \sin[k_0 Q_n(t_{j'})] &= \hbar k_0^2 g(t_{j'} - t_j) \cos[k_0 Q_0(t_{j'})] + O\left[\left[\frac{\hbar k_0^2 g_{\max}}{2}\right]^3\right] \\ &= \hbar k_0^2 \left[\frac{\delta Q_0(t_{j'})}{\delta \xi(t_j)}\right] \cos[k_0 Q_0(t_{j'})] + O\left[\left[\frac{\hbar k_0^2 g_{\max}}{2}\right]^3\right] \\ &= \hbar k_0 \left[\frac{\delta}{\delta \xi(t_j)} \sin[k_0 Q_0(t_{j'})]\right] + O\left[\left[\frac{\hbar k_0^2 g_{\max}}{2}\right]^3\right] . \end{aligned}$$

The general case can be done in the same way.

Using (5.9) and putting $V_0 k_0 \sin(k_0 Q) = -V_a'(Q)$ into (2.30) [see (2.19)] we obtain

$$\begin{aligned} w(Q_f, P_f, t) = \Bigg\langle & \delta(Q_f - Q_0)\delta(P_f - P_0(t)) \\ & + \sum_{n=1}^{\infty} \left[\frac{-1}{\hbar}\right]^n \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \times \hbar V_a'(Q_0(t_1)) \frac{\delta}{\delta \xi(t_1)} \\ & \times \left[\cdots \left[\hbar V_a'(Q_0(t_n)) \frac{\delta}{\delta \xi(t_n)} \times [\delta(Q_f - Q_0(t))\delta(P_f - P_0(t))] \right] \cdots \right] \Bigg|_{\{\sigma_j = 0\}} \Bigg\rangle \\ & + O\left[\left[\frac{\hbar k_0^2 g_{\max}}{2}\right]^3\right] \\ = \Bigg\langle & \exp\left[-\int_0^t d\tau\, V_a'(Q_0(\tau)) \frac{\overleftrightarrow{\delta}}{\delta \xi(\tau)}\right] \delta(Q_f - Q_0(t))\delta(P_f - P_0(t)) \Bigg\rangle + O\left[\left[\frac{\hbar k_0^2 g_{\max}}{2}\right]^3\right] , \end{aligned} \qquad (5.10)$$

where in the last step we have used the fact that

$$\frac{\delta Q_0(\tau)}{\delta \xi(\tau')} = 0 \quad \text{for } \tau < \tau'$$

so that the series can be summed up. Since (5.10) agrees exactly with (5.5), it is clear that (5.7) gives a more precise criterion for the quasiclassical approximation. Note that for $\eta \to 0$, $g_{\max} \to 1/(M\omega_0)$; while for $\eta \to \infty$, $g_{\max} \sim 1/\eta$, making (5.7) nearly the same as (5.3) in that limit (taking here $L_0 \sim 1/k_0$).

It is interesting to note that the criteria (5.3) and (5.7) are obtained from different effects of the environment; the former comes from the fluctuation whereas the latter comes from the dissipation. Moreover, in the limit $\hbar \to 0$, (5.10) is exact and the spectrum of the noise becomes "white;" we then fully recover the classical Langevin equation.

The quasiclassical approximation *violates* the important Green-Kubo-Einstein relation which relates the linear mobility and diffusion constant. This will be seen in the next section [cf. Refs. 6 and 10; keeping only $\hbar$ in $C(t)$, which is precisely what the quasiclassical approximation does, invalidates the identity]. Note also that our argument is restricted to fixed finite times. As the time increases, the ignored contributions may become significant. Consequently, it is not clear whether it is legitimate to apply it in tunneling problems (cf. Ref. 19).

VI. SOME CONNECTIONS TO THE JOSEPHSON JUNCTION

A. Washboard potential and Einstein relation

The anharmonic potential in (2.18) and (2.19b) corresponds to that of a single Josephson tunnel junction, see, e.g., Ref. 20. If the quadratic part of (2.19a) vanishes while the external field F (i.e., the external current through the junction) is different from zero, the particle will slide down the "washboard" potential and eventually move with a constant average velocity. An important quantity in practice is the mobility of the particle. This problem has been studied by several authors.[10–12] In particular, our approach using (2.30) and (2.31) is similar to Fisher and Zwerger[10] but with some differences in the way of performing the path integration which we believe makes it more physically transparent.

We shall focus our attention on the Einstein relation which links the linear mobility ν and the diffusion constant D via $D=kT\nu$. Although Kubo[21] has given a formal derivation of the linear-response theory to which the Einstein relation belongs, there are some problems here with the definition of ν arising from the fact that the stationary state in which the particle moves with a constant velocity is not normalizable. To get over these problems in the classical system one has to define the measure on the environment as seen by the particle (the so-called Palm measure[22]) which is stationary whenever the medium in which the particle moves is translationally invariant e.g., a homogeneous random environment (this includes the periodic case). Alternatively, one can use, for a periodic potential, a finite box with the same periodicity and compute the stationary distribution of the particle in that box. This will then give the same answer for the velocity distributions as the infinite system. Unfortunately, neither of these prescriptions works for quantum systems because we cannot define appropriately the Palm measure and the equivalence for a periodic potential between an infinite system and a finite periodic box does not hold due to the requirement of periodicity of the wave functions in the latter case. We are therefore forced to consider an initial state in which the particle is localized near the origin and then define the mean velocity in the presence of an external field $\bar{v}(F)$ as

$$\bar{v}(F)=\lim_{t\to\infty}\langle \dot{Q}(t)\rangle_F=\lim_{t\to\infty}\frac{\langle Q(t)\rangle_F}{t},$$

assuming that the limit in fact exists. The linear mobility ν is given by $\nu=\lim_{F\to 0}[\bar{v}(F)/F]$. The advantage and disadvantage of this definition of ν is that we neither require nor obtain any information about the stationary distribution in the presence of a field F—except for the assumption of the existence of the two limits. There is, however, also a question now about the applicability of the general derivation of linear-response theory, so it is useful to investigate the Einstein relation explicitly for the quantum system. In particular, it is not obvious *a priori* whether $D\to 0$ or $\nu\to\infty$ (or both) as $T\to 0$.

The so-called RSJ (resistively shunted junction) model[20] corresponds here to Ohmic damping with infinite cutoff where the Green's function $g(\tau)$ entering (2.30) has the simple form

$$g(\tau)=\Theta(\tau)\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\eta\sin(\omega\tau)}{\omega(M^2\omega^2+\eta^2)}=\frac{\Theta(\tau)}{\eta}\left[1-\exp\left[-\frac{\eta}{M}\tau\right]\right]. \tag{6.1}$$

It is then straightforward to obtain from (2.30) and (2.31) the exact formal expression for the diffusion constant

$$D=\lim_{t\to\infty}\frac{\langle Q(t)^2\rangle}{2t},$$
$$D=D_0+2kT(\nu-\nu_0)-\sum_{n=1}^{\infty}(-1)^nV_0^{2n}\int_{-\infty}^{0}dt_{2n-1}\cdots\int_{-\infty}^{t_2}\sum_{\{\mu_j=\pm1\}}\frac{k_0^2}{4\hbar}\sum_{l=1}^{2n-1}\text{cotan}\left[\frac{\hbar k_0^2}{2}\sum_{j=l+1}^{2n}\mu_j g(t_j-t_l)\right]\times F_1(\{t_j,\mu_j\})F_2(\{t_j,\mu_j\})\Big|_{t_{2n}=\sum_j^{2n}\mu_j=0}, \tag{6.2}$$

where $D_0=kT\nu_0=kT/\eta$ and ν is the linear mobility given by

$$\nu=\frac{1}{\eta}+\frac{k_0^2}{2\eta^2}\sum_{n=1}^{\infty}(-1)^nV_0^{2n}\int_{-\infty}^{0}dt_{2n-1}\cdots\int_{-\infty}^{t_2}\sum_{\{\mu_j=\pm1\}}\left[\sum_{l=1}^{2n}\mu_l t_l\right]F_1(\{t_j,\mu_j\})F_2(\{t_j,\mu_j\})\Bigg|_{t_{2n}=\sum_j^{2n}\mu_j=0}. \tag{6.3}$$

The functions F_1 and F_2 entering (6.2) and (6.3) have the form

$$F_1(\{t_j,\mu_j\})=\prod_{k=1}^{2n-1}\frac{1}{\hbar}\sin\left[\frac{\hbar k_0^2}{2}\sum_{j=k+1}^{2n}\mu_j g(t_j-t_k)\right], \tag{6.4}$$

$$F_2(\{t_j,\mu_j\})=\exp\left[\frac{k_0^2}{2}\sum_{j,k=1}^{2n}\mu_j\mu_k C(t_j-t_k)\right], \tag{6.5}$$

where $C(t)$ is the "mean-square displacement" after a "long time"

$$C(t)=\lim_{t'\to\infty}\langle[Q_0(t+t')-Q_0(t')]^2\rangle/2=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\eta\omega\hbar\left[\coth\frac{\beta\omega\hbar}{2}\right]\frac{1-\cos(\omega t)}{\omega^2(M^2\omega^2+\eta^2)}. \tag{6.6}$$

Equations (6.2) and (6.3) are formally exact expressions for the mobility and the diffusion constant. In particular, taking $\hbar \to 0$, they coincide, as proved in Sec. IV, with those obtained from solving the classical Langevin equation where the Einstein relation has been proven rigorously to all orders.[22]

The verification of the Einstein relation to the lowest order in (6.2) and (6.3) is also remarkably easy. In fact. we have

$$\nu = \nu_0 - \left[\frac{V_0 k_0}{\eta}\right]^2 \int_0^\infty dt \frac{t}{\hbar} \sin\left[\frac{\hbar k_0^2}{2} g(t)\right] \times \exp\left[-C(t)\left[\frac{2\pi}{q_0}\right]^2\right] + O(V_0^4) \tag{6.7}$$

and

$$D = 2kT(\nu - \nu_0) + kT/\eta + \frac{1}{2}\left[\frac{V_0 k_0^2}{\eta}\right]^2 \int_0^\infty dt \cos\left[\frac{\hbar k_0^2}{2} g(t)\right] \times \exp[-k_0^2 C(t)] + O(V_0^4) \ . \tag{6.8}$$

The Einstein relation then follows immediately from the following identity:

$$2kT \int_0^\infty dt \frac{t}{\hbar} \sin\left[\frac{\hbar k_0^2}{2} g(t)\right] \exp[-k_0^2 C(t)] \equiv \int_0^\infty dt \cos\left[\frac{\hbar k_0^2}{2} g(t)\right] \exp[-k_0^2 C(t)] \ . \tag{6.9}$$

The proof of (6.9) was given in the appendix of Fisher and Zwerger[10] and is related to the detailed balance condition between forward and backward hopping. Unfortunately, higher orders are not so simple and hence much harder work needs to be done.

It is interesting to note that the duality transformation for the diffusion constants between the continuous periodic potential and tight binding limit (TB) now involves both D and ν. In fact by comparing (6.2)–(6.6) with the result of Weiss and Wollensak,[12] we find

$$D = \nu_0 + D_{\rm TB} - 2kT\nu_{\rm TB} \ , \tag{6.10}$$

with the appropriate parameter mappings discussed in Fisher and Zwerger.[10] Not surprisingly when the Einstein relation holds *exactly* in one case it does so also in the other case. Note that Weiss and Wollensak have, working on the tight-binding model, summed over the higher-order terms and proved the Einstein relation in certain limits. Nevertheless, the approximations made there do not seem appropriate when one maps them to our case.

B. The time evolution of a rf SQUID

A Josephson junction with its two leads joined into a superconducting ring is called a rf SQUID.[20] With appropriate choices of the SQUID's parameters, many interesting potentials can be obtained such as a double well or a metastable potential; both of these have been widely used in many fields (cf. Ref. 3).

Our particular interest here is to develop an expression for the quantum-mechanical time evolution of the system, starting with the physically appropriate mixed initial state. This avoids the artificial transient behavior induced by the product initial state (cf. Refs. 3–5). Furthermore, we are interested only in the positional quantities of the particle, so that the cutoff of the spectrum can be simply removed. Using the equivalence established in Sec. III B and Appendix B, we start the evolution of the system at $t = -\infty$ in the initial potential

$$V_i(\hat{x}) = \tfrac{1}{2} M\Omega_0(\hat{x} - q_i)^2 \tag{6.11}$$

and then switch at $t = 0$ to the true potential described by (2.18) and (2.19) (setting the field $F = 0$ for simplicity). Note that the parameters q_i and Ω_0 should be chosen according to the position and the oscillating frequency of the starting well. The general expression (2.30) for the Wigner distribution will remain correct for $t > 0$ provided $Q_n(\tau)$ is obtained from the following Langevin equation (with sources):

$$M\ddot{Q} + \eta\dot{Q} + M\Omega_0^2(Q - q_i) = \xi(\tau), \quad -\infty < \tau < 0 \ , \tag{6.12a}$$

$$M\ddot{Q} + \eta\dot{Q} + M\omega_0^2 Q = \xi(\tau) + \frac{\pi\hbar}{q_0}\sum_{j=1}^{n} \sigma_j g(\tau - t_j), \quad \tau > 0 \ . \tag{6.12b}$$

To average over the random noise we introduce the modified "frequency"

$$\tilde{\omega} = \left[\left[\frac{\eta}{2M}\right]^2 - \omega_0^2\right]^{1/2} , \tag{6.13}$$

which can be either real or imaginary. Then the Green's function for $\tau > 0$ [see (2.29)] has the simple form

$$g(\tau) = \Theta(\tau) \exp\left[\frac{-\eta\tau}{2M}\right] \frac{\sinh(\tilde{\omega}\tau)}{\tilde{\omega}} \ . \tag{6.14}$$

After some straightforward manipulations, we obtain

$$\langle Q(t)\rangle = q_i X(t) + \frac{1}{2}\left[\frac{2\pi}{q_0}\right] \sum_{n=1}^{\infty} V_0^n \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 S_n(t_n, t_{n-1}, \ldots, t_1) \ , \tag{6.15}$$

where $X(\tau)$ is the trajectory of the particle starting with $Q(0) = 1$, $\dot{Q}(0) = 0$,

$$X(\tau) = \Theta(\tau)\left[\frac{\omega_+ e^{-\omega_-\tau} - \omega_- e^{-\omega_+\tau}}{\omega_+ - \omega_-}\right], \quad \omega_\pm = -\frac{\eta}{2M} \pm \tilde{\omega} \tag{6.16a}$$

and

$$S_n(t_n,t_{n-1},\ldots,t_1)=g(t-t_n)\sum_{\{\mu_j=\pm1\}}\sin\left[\mu_1 k_0\sum_{k=1}^{n}\mu_j[q_i X(t_j)-b]\right]\left[\prod_{k=1}^{n-1}\frac{1}{\hbar}\sin\left[\frac{\hbar\mu_{k+1}k_0^2}{2}\sum_{l=k+1}^{n}\mu_l g(t_l-t_k)\right]\right]\times\exp\left[-\frac{k_0^2}{2}\sum_{J,k=1}^{n}\mu_j\mu_k C(t_j,t_k)\right]. \qquad (6.16b)$$

In (6.16b), $C(\tau,\tau')$ is the correlation function

$$C(\tau,\tau')=\langle Q_0(\tau)Q_0(\tau')\rangle=\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{\eta\hbar\coth(\beta\hbar\omega/2)}{M^2(\omega_0^2-\omega^2)^2+\eta^2\omega^2}\{\cos[\omega(\tau-\tau')]+\cdots\}, \qquad (6.17)$$

where the transient parts, represented by the ellipsis, can be obtained from (6.12) (but are rather messy).

Having obtained a well-defined dissipative quantum evolution of the system *starting with the mixed initial state,* we still need to carry out the multidimensional integrals associated with the expansion in powers of V_0. If both V_0 and t are small, numerical evaluations of the first few coefficients of V_0 should be quite adequate [using either (6.16) or starting with the Langevin equations (6.12)] but we have not found an effective (either numerical or analytical) method for the general case when the time t becomes larger. We note, however, that (6.15) and (6.16) have a similarity with the expansion for a two-state system in Ref. 3 so a similar analysis can perhaps also be carried out here. An important difference is that the odd powers in Δ (the tunneling matrix element) do not appear there. This might be an indication that some information is lost when we discretize the continuous system (bearing in mind the formal mapping $V_0\to\Delta$ for the case of periodic potential[10,12]).

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APPENDIX A: PATH-INTEGRAL FORMALISM

In this appendix we derive the path-integral representation for the transformation $J_\alpha(Q_f,r_f,t;Q_i,r_i,0)$ ($\alpha=P$ or M) defined in (2.9). We need to evaluate for the product initial state

$$J_P(x,y,t;x',y',0)=\frac{\mathrm{Tr}_e(e^{-\beta\hat H_e}\langle y'|e^{i\hat Ht/\hbar}|y\rangle\langle x|e^{-i\hat Ht/\hbar}|x'\rangle)}{\mathrm{Tr}_e(e^{-\beta\hat H_e})} \qquad (A1)$$

and for the mixed initial state

$$J_M(x,y,t;x',y',0)=\frac{\mathrm{Tr}_e(\langle x'|e^{-\beta\hat H}|y'\rangle\langle y'|e^{i\hat Ht/\hbar}|y\rangle\langle x|e^{-i\hat Ht/\hbar}|x'\rangle)}{\mathrm{Tr}_e(e^{-\beta\hat H_e})}, \qquad (A2)$$

where we have used for convenience

$$x=Q_f+r_f/2,\quad y=Q_f-r_f/2;\quad x'=Q_i+r_i/2,\quad y'=Q_i-r_i/2. \qquad (A3)$$

To introduce the path integrals, we define a contour γ which starts at the origin and goes from $\tau=0+i\epsilon$ to $\tau=t+i\epsilon$ (γ_{I}), then from $\tau=t-i\epsilon$ back to $\tau=0-i\epsilon$ (γ_{II}), and finally from $\tau=0-i\epsilon$ to $-i\beta\hbar$ (γ_{III}); see Fig. 1 (ϵ being infinitesimal). We further define a time-order operator $\hat T_\gamma$ along γ for the environment. We can now express the evolution of the particle in terms of path integrals while treating the environmental part by the usual time-ordering technique. It is straightforward to show ($\alpha=P$ or M)

$$J_\alpha(x,y,t;x',y',0)=\int\mathcal{D}z(\tau)\exp\left[i\int_{\gamma_\alpha}d\tau\left[\frac{M}{2}\dot z^2-V(z)\right]\right]F_\alpha[z(\tau)], \qquad (A4)$$

where

$$F_P[z(\tau)]=\frac{\mathrm{Tr}_e\left[\exp(-\beta\hat H_e)\hat T_\gamma\exp\left[-\frac{i}{\hbar}\int_{\gamma_P}d\tau\sum_k[\hbar\omega_k\hat a_k^\dagger\hat a_k+C_k(\hat a_k+\hat a_k^\dagger)z+C_k^2z^2/(\hbar\omega_k)]\right]\right]}{\mathrm{Tr}_e(e^{-\beta\hbar_e})}, \qquad (A5a)$$

$$F_M[z(\tau)]=\frac{\mathrm{Tr}_e\left[\hat{T}_\gamma\exp\left[-\frac{i}{\hbar}\int_{\gamma_M}d\tau\sum_k[\hbar\omega_k\hat{a}_k^\dagger\hat{a}_k+C_k(\hat{a}_k+\hat{a}_k^\dagger)z+C_k^2z^2/(\hbar\omega_k)]\right]\right]}{\mathrm{Tr}_e(e^{-\beta\hat{H}_e})} . \tag{A5b}$$

Note that $\gamma_P=\gamma_{\rm I}+\gamma_{\rm II}$ whereas $\gamma_M=\gamma$ with $V(z(\tau))\equiv V_i(z(\tau))$ for $\tau\in\gamma_{\rm III}$. The dependence of the right side of (A4) on (x,y) and (x',y') is implicit through the boundary conditions

$$z(0+i\epsilon)=z(-i\beta\hbar)=x',\quad z(t+i\epsilon)=x\ ;$$
$$z(0-i\epsilon)=y',\quad z(t-i\epsilon)=y\ .$$

The trace over the environmental degrees of freedom [on the right sides of (A5)] can be readily done. To see this let us introduce the Heisenberg representation:

$$\hat{a}_k(\tau)=e^{i\tau\hat{H}_e/\hbar}\hat{a}_k e^{-i\tau\hat{H}_e/\hbar} ,$$
$$\hat{a}_k^\dagger(\tau)=e^{i\tau\hat{H}_e/\hbar}\hat{a}_k^\dagger e^{-i\tau\hat{H}_e/\hbar} . \tag{A6}$$

Using (A6) we can rewrite (A5) as

$$F_\alpha[z(\tau)]=\frac{\mathrm{Tr}_e\left[\exp(-\beta\hat{H}_e)T_\gamma\exp\left[-\frac{i}{\hbar}\int_{\gamma_\alpha}d\tau\sum_k C_k[\hat{a}_k(\tau)+\hat{a}_k^\dagger(\tau)]z(\tau)\right]\right]}{\mathrm{Tr}_e\exp(-\beta\hat{H}_e)}\exp\left[-\frac{i}{\hbar}\int_{\gamma_\alpha}d\tau\sum_k\frac{C_k^2z^2}{\hbar\omega_k}\right] , \tag{A7}$$

where $\alpha=P$ or M. This is a standard expression for the so-called generating functional.[23] Note that the thermal average over the bath states is simply a Gaussian measure. Therefore, the result can be put in a compact form[23] (via, e.g., standard Green's function or path-integral techniques):

$$F_\alpha[z(\tau)]=\exp\left[-\frac{i}{\hbar^2}\int_{\gamma\alpha}d\tau\,d\tau'\sum_k\left[z(\tau)C_k^2G_k(\tau,\tau')z(\tau')+\frac{C_k^2z^2}{\omega_k}\right]\right] , \tag{A8}$$

where $G_k(\tau,\tau')$ is the covariance of the Gaussian measure or the Green's function of the "phonons,"

$$G_k(\tau,\tau')=-i\hbar\frac{\mathrm{Tr}_e\{e^{-\beta\hat{H}_e}T_\gamma[\hat{a}_k(\tau)\hat{a}_k^\dagger(\tau')]\}}{\mathrm{Tr}_e(e^{-\beta\hat{H}_e})}$$
$$=-i\hbar\left[\Theta_\gamma(\tau,\tau')+\frac{1}{\exp(\beta\hbar\omega_k)-1}\right]$$
$$\times\exp[-i\omega_k(\tau-\tau')] . \tag{A9}$$

The function $\Theta_\gamma(\tau,\tau')$ in (A9) is the step function along γ, i.e., $\Theta_\gamma(\tau,\tau')=1$ if τ is "after" τ'; otherwise it is zero.

APPENDIX B: MIXED INITIAL STATE

1. Path integration over the imaginary axis

In the first part of this appendix we shall carry out the path integral (2.12b). Note that one needs to be very careful about using the Fourier transform since the boundary conditions are asymmetric. It is convenient to change the integral into a new one with zero-boundary conditions. To do this we introduce the following variable transformation:

$$q(\tau)=\tilde{q}(\tau)+\delta q(\tau) , \tag{B1a}$$

where

$$\delta q(\tau)\equiv Q_i+r_i\frac{(\tau-\beta\hbar/2)}{\beta\hbar} \tag{B1b}$$

so that $\tilde{q}(0)=\tilde{q}(\beta\hbar)=0$. To express the action (2.13b) in terms of the new variable $\tilde{q}(\tau)$, we have to treat the kinetic energy separately,

$$\frac{M}{2\hbar}\int_0^{\beta\hbar}d\tau\,\dot{q}^2(\tau)=\frac{M}{2\hbar}\int_0^{\beta\hbar}d\tau\,\dot{\tilde{q}}^2(\tau)+\frac{Mr_i^2}{2\beta\hbar^2} . \tag{B2}$$

The remaining terms are well behaved and can be accordingly expressed in terms of the Fourier transform of $\tilde{q}(\tau)$. Thus, the action (2.13b) becomes

$$S[\tilde{q}(\tau)]=\beta\sum_{n=-\infty}^{\infty}[K_n|\tilde{q}_n|^2/2$$
$$+\tilde{q}_n(\tilde{K}_n\delta q_{-n}-if_n/\beta)]+S_0 , \tag{B3}$$

with

$$S_0=\beta\sum_{n=-\infty}^{\infty}(\tilde{K}_n|\delta q_n|^2/2-i\delta q_nf_n/\beta)+\frac{Mr_i^2}{2\beta\hbar^2} , \tag{B4}$$

where

$$\delta q_n=\frac{ir_i}{\beta\hbar\nu_n}\ \text{ for } \nu_n\neq0,\quad \delta q_n=Q_i\ \text{ for } \nu_n=0 , \tag{B5}$$

and

$$\tilde{K}_n=K_n-M\nu_n^2 . \tag{B6}$$

Let us first consider the following generating functional for the partition function:

$$G(\{\lambda_n\})=\int_{q(0)=q(\beta)}\mathcal{D}q(\tau)\exp\left[-\beta\sum_{n=-\infty}^{\infty}K_n|q_n|^2/2-\lambda_n q_n\right]. \quad \text{(B7a)}$$

We can carry out the path integration by simply completing the squares in the exponent. This yields

$$G(\{\lambda_n\})=Z_r\exp\left[\frac{1}{2}\sum_{n=-\infty}^{\infty}\frac{\lambda_n\lambda_{-n}}{\beta K_n}\right], \quad \text{(B7b)}$$

where Z_r is the reduced partition function of the particle (see Sec. II A for the definition). From (B7b) it is easy to find the equilibrium covariance of the harmonic system

$$W(\tau)=\langle q(\tau)q(0)\rangle_0=\sum_{n=-\infty}^{\infty}\frac{e^{i\nu_n\tau}}{\beta K_n}, \quad \text{(B8)}$$

which is used in Sec. III B. We now replace the periodic boundary condition by the zero-boundary condition considered here, $\tilde{q}(0)=\tilde{q}(\beta\hbar)=0$. This can be done by multiplying the integrand of (B7) (setting $q\to\tilde{q}$) by the δ function

$$\delta(\tilde{q}(0))=\delta(\tilde{q}(\beta\hbar))=\int_{-\infty}^{\infty}\frac{d\lambda}{2\pi}\exp\left[-i\lambda\beta\sum_{n=-\infty}^{\infty}\tilde{q}_n\right]. \quad \text{(B9)}$$

We then have the modified generating functional

$$\tilde{G}(\{\lambda_n\})=\frac{Z(\beta)}{\sqrt{2\pi W(0)}}=\left[\frac{1}{2}\sum_{n=-\infty}^{\infty}\frac{\lambda_n\lambda_{-n}}{\beta K_n}-\frac{1}{2W(0)}\left[\sum_{-\infty}^{\infty}\frac{\lambda_n}{\beta K_n}\right]^2\right]. \quad \text{(B10)}$$

Taking $\lambda_n=(\beta\tilde{K}_n\delta q_{-n}-if_n)$ [according to (B3)] and after some manipulations, we obtain finally the result (2.14).

2. Equivalence to the product state in the ohmic limit

Taking the ohmic damping limit (3.1) and (3.2), we can reduce (2.13c) and (2.13d) to the following forms:

$$K_n=M\nu_n^2+M\omega_0^2+\frac{\eta|\nu_n|\omega_c}{\omega_c+|\nu_n|}, \quad \text{(B11a)}$$

$$f_n=\frac{\eta}{\hbar}\int_0^t ds\, r(s)\left[\frac{2\theta(-\nu_n)\nu_n\omega_c^2\exp(-\nu_n s)+(\omega_c-\nu_n)\exp(-\omega_c s)}{\omega_c^2-\nu_n^2}\right]. \quad \text{(B11b)}$$

Using (B11a), we have the two covariances [see (2.14b)]

$$\sigma_x=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\frac{\omega_c+|\nu_n|}{P(|\nu_n|)}, \quad \text{(B12a)}$$

and

$$\sigma_p=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\frac{(M\omega_0^2+\eta\omega_c)|n_n|+M\omega_0^2\omega_c}{P(|\nu_n|)}, \quad \text{(B12b)}$$

where

$$P(\nu)=M\nu^3+M\omega_c\nu^2+(\eta\omega_c+M\omega_c^2)\nu+M\omega_0^2\omega_c; \quad \text{(B12c)}$$

the other quantities on the right side of (2.14a) will also be given below.

Now if all the zeros of $P(-i\nu)$ lie below the real axis, which is equivalent to the requirement that all the eigenmodes of the equation of motion (2.21) are exponentially damped (in our case this is always true), the sum over the discrete Fourier frequencies ν_n in (B12) can be converted into a continuous integral via an appropriate contour integration closing the upper half-plane of ν. It is then not difficult to find

$$\sigma_x=\mathrm{Im}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\hbar(\omega_c-i\omega)\coth(\beta\hbar\omega/2)}{P(-i\omega)}=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\eta\hbar\omega\coth(\beta\hbar\omega/2)}{|P(-i\omega)|^2/\omega_c^2} \quad \text{(B13a)}$$

and

$$\sigma_p=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{M^2\eta\hbar\omega^3\coth(\beta\hbar\omega/2)}{|P(-i\omega)|^2/\omega_c^2}, \quad \text{(B13b)}$$

which agree with the real-time result (3.8). The expressions for other quantities in (2.14a) are more complicated. Introducing the function

$$Y(\omega)=\frac{J(\omega)(\omega_c-i\omega)\hbar\coth(\beta\hbar\omega/2)}{P(-i\omega)}, \quad \text{(B14)}$$

we then obtain

$$i\sum_{n=-\infty}^{\infty}\frac{f_n}{\beta K_n}=i\int_0^t\frac{ds}{\hbar}r(s)\left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}Y(\omega)\left[\exp(i\omega s)+\frac{\omega_c}{i\omega}\exp(-\omega_c s)\right]\right] \quad \text{(B15a)}$$

$$\sum_{n=-\infty}^{\infty}\frac{f_n f_{-n}}{\beta K_n}=\left[\eta\int_0^t\frac{ds}{\hbar}r(s)\omega_c\exp(-\omega_c s)\right]\int_0^t\frac{ds}{\hbar}r(s)\left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}Y(\omega)\left[\frac{2\omega_c\exp(i\omega s)}{\omega_c-i\omega}+\frac{\omega_c}{i\omega}\exp(-\omega_c s)\right]\right], \tag{B15b}$$

and

$$\sum_{n=-\infty}^{\infty}\frac{Mf_n\nu_n}{\beta K_n}=-i\int_0^t\frac{ds}{\hbar}r(s)\left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}M\omega Y(\omega)[\exp(i\omega s)+\exp(-\omega_c s)]\right]. \tag{B15c}$$

In what follows, we shall rederive these results by extending the initial time of the product state, say t_i, to $-\infty$. Note that we can decompose the effective action (2.17) [but not using the trick (2.15)] with initial time $t_i<0$ into three parts

$$\frac{i}{\hbar}S_{\rm tot}=\frac{i}{\hbar}(S_1+S_2+S_{12}), \tag{B16}$$

where S_1 is the action starting at time $t=0$ and

$$\frac{i}{\hbar}S_2=\frac{i}{\hbar}M\dot{r}Q\Big|_{t_i}^{0}-\frac{i}{\hbar}\int_{t_i}^{0}d\tau\left[M\ddot{r}+M\omega_0^2 r+\alpha_1(\tau)r(0)-\int_{\tau}^{\theta}d\tau'\alpha_1(\tau'-\tau)\dot{r}(\tau)\right]Q(\tau)-\frac{1}{2\hbar^2}\int_{t_i}^{0}d\tau\,d\tau' r(\tau)\alpha_2(\tau-\tau')r(\tau'), \tag{B17a}$$

$$\frac{i}{\hbar}s_{12}=-\frac{i}{\hbar}\int_0^t ds\,r(s)\int_{t_i}^{2}d\tau\,\dot{\alpha}_1(s-\tau)Q(\tau)-\int_0^t ds\,r(s)\int_{t_i}^{0}d\tau\,\alpha_2(s-\tau)r(\tau). \tag{B17b}$$

We can now integrate out of $Q(\tau)$ with $\tau<0$ which, in analogue to the integration over $r(\tau)$ in Sec. II C, results in an equation of motion for the other variable $r(\tau)$,

$$M\ddot{r}+M\omega_0^2 r-\int_{\tau}^{0}d\tau'\alpha_1(\tau'-\tau)\dot{r}(\tau')+\alpha_1(\tau)r(0)+\int_0^t ds\,r(s)\dot{\alpha}_1(s-\tau)=0. \tag{B18}$$

The solution of $r(\tau)$ will decay backwards in time. Let us define

$$\tilde{r}(\omega)=\int_{-\infty}^{0}d\tau\,r(\tau)e^{-i\omega\tau}. \tag{B19}$$

Then (B18) gives

$$\tilde{r}(\omega)=\{\omega_c R-M(\omega_c-i\omega)[\dot{r}(0)+i\omega r(0)]\}/P(-i\omega), \tag{B20a}$$

where

$$R=\int_0^t ds\,r(s)\eta\omega_c e^{-\omega_c s}. \tag{B20b}$$

Now the contribution from $\tau<0$ to the remaining effective action beginning at $\tau=0$ is, if we put in (B17) $t_i\to-\infty$ and substitute (B20) into the rest of the terms associated with $r(\tau)$ $(\tau<0)$,

$$i\Delta s=iQ(0)\frac{M\dot{r}}{\hbar}-\frac{1}{2\hbar^2}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\tilde{J}(\omega)\left[|\tilde{r}(\omega)|^2+2\int_0^t ds\,r(s)\tilde{r}(\omega)e^{i\omega s}\right] \tag{B21a}$$

with

$$\tilde{J}(\omega)=J(\omega)\hbar\coth\left[\frac{\beta\hbar\omega}{2}\right]. \tag{B21b}$$

Straightforward manipulations give

$$\Delta S=-\frac{\sigma_x M^2\dot{r}^2(0)}{2\hbar^2}-\frac{\sigma_p r^2(0)}{2\hbar}+\frac{M\dot{r}}{\hbar}A+i\frac{Mr(0)}{\hbar}B-C, \tag{B22}$$

where

$$A=iQ(0)+\frac{\omega_c^2 R}{\hbar}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\tilde{J}(\omega)}{|P(-i\omega)|^2}+\int_0^t\frac{ds}{\hbar}r(s)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\tilde{J}(\omega)(\omega_c-i\omega)}{P(-i\omega)}\exp(i\omega s), \tag{B23a}$$

$$B=\int_0^t\frac{ds}{\hbar}r(s)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\tilde{J}(\omega)(\omega_c-i\omega)}{P(-i\omega)}\exp(i\omega s)=i\frac{\omega_c R}{\hbar}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\tilde{J}(\omega)\omega^2}{|P(-i\omega)|^2}, \tag{B23b}$$

and

$$C=\frac{\omega_c^2R^2}{2\hbar^2}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\tilde{J}(\omega)}{|P(-i\omega)|^2}+\frac{\omega_c R}{\hbar}\int_0^t\frac{ds}{\hbar}r(s)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\tilde{J}(\omega)}{P(-i\omega)}\exp(i\omega s)\ . \tag{B23c}$$

The quantities B and C have already been shown to agree with the corresponding imaginary time result (B15b) and (B15c).

We have to eventually integrate over the initial configuration (Q_i,r_i) at time t_i. The integration over Q_i is simply 1, due to the normalization of the initial state, while the integration over r_i can be transformed to the integration over $M\dot{r}(0)/\hbar$. It is shown in Appendix C (for this case, viewing the time flowing backwards) that the Jacobian of this transformation cancels exactly with another one arising from the elimination of the intermediate paths of $r(\tau)$. Carrying out this integration, we then fully recover the imaginary-time result. Note also that, since the solution of (B18) decays backwards in time exponentially, we can, at $t_i\to\infty$, simply set $r_i=0$ in the initial density matrix.

APPENDIX C: JACOBIAN OF THE PATH INTEGRATION OVER $Q(\tau)$

In certain cases (most appropriately the strong damping limit), one can approximately linearize the effective action (2.17) (cf. Secs. II and V) with respect to $r(\tau)$ and then carry out $\int\mathcal{D}r(\tau)$ in (2.16). This leads to the requirement that the other variable $Q(\tau)$ is restricted to the solution of the c-number quantum Langevin equation, see (2.20) and (2.21) with $V_h(x)$ replaced by the general potential $V(x)$. In this appendix we shall compute the Jacobian resulting from the path integration over $Q(\tau)$. We start with the discretized version of the path integral[15] [see (2.20)],

$$J(Q_f,r_f,t;Q_i,r_i,0)=\frac{1}{2\pi\hbar}\left[\frac{M}{\epsilon}\right]^N\int_{-\infty}^{\infty}\left[\prod_{k=1}^{N-1}dQ_k\right]\left[\prod_{k=1}^{N-1}\delta(Y_k)\right]\exp\left[i\frac{Mr_f(Q_f-Q_{N-1})}{\epsilon\hbar}-i\frac{Mr_i(Q_1-Q_i)}{\epsilon\hbar}\right]$$
$$=\exp\left[\frac{i}{\hbar}M(r_f\dot{Q}_f-r_i\dot{Q}_i)\right]\Big/|D_{N-1}|\ , \tag{C1}$$

where the new variable Y_k is given by

$$Y_k=-M\frac{Q_{k+1}-2Q_k+Q_{k-1}}{\epsilon}-\epsilon V'(Q_k)+\epsilon\xi_k-\epsilon\sum_{m=1}^{k}(Q_m-Q_{m-1})\alpha_1(k\epsilon-m\epsilon)-\epsilon\alpha_1(k\epsilon)Q_i \tag{C2}$$

and D_{N-1} is the Jacobian to be computed,

$$D_{N-1}=2\pi\hbar\left[\frac{\epsilon}{M}\right]^N\left|\frac{\partial(Y_1,Y_2,\ldots,Y_{N-1})}{\partial(Q_1,Q_2,\ldots,Q_{N-1})}\right|\ . \tag{C3}$$

The problem has now been reduced to the evaluation of the determinant. Writing it out explicitly, one can find that it is nearly upper triangular. Thus, we shall try to search for a recursion relation which links D_n with $D_{n-1},\ldots,D_1$, where D_n is the truncated determinant in which we take the first $n\times n$ matrix elements. Indeed, it turns out that

$$D_{n+1}=\left[2-\frac{\epsilon^2}{M}V''(Q_{n+1})-\frac{\epsilon^2\alpha_1(0)}{M}\right]D_n+\left[-1+\sum_{k=1}^{n-1}\frac{\epsilon^2}{M}[\alpha_1((k-1)\epsilon)-\alpha_1(k\epsilon)]D_{n-k}\right]\ . \tag{C4}$$

This can be expressed in a more familiar form

$$\frac{D_{n+1}-2D_n+D_{n-1}}{\epsilon^2}+\frac{V''(Q_{n+1})}{M}+\sum_{k=0}^{n-2}\frac{\alpha_1(k\epsilon)}{M}(D_{n-k}-D_{n-k-1})+D_1\alpha_1((n-1)\epsilon)=0\ , \tag{C5}$$

which in the continuous limit ($\epsilon\to 0$) reduces to the equation of motion for the quantity $\partial Q/\partial Q_i$ [cf. (2.21)],

$$M\ddot{D}+\int_0^\tau d\tau'\dot{D}(\tau')\alpha_1(\tau')+V''(Q(\tau))D=0\ . \tag{C6}$$

We now check the initial conditions for both of the quantities. For $\partial Q/\partial Q_i$, we have

$$\left.\frac{\partial Q}{\partial \dot{Q}_i}\right|_{\tau=0}=0,\quad \left.\frac{d}{d\tau}\left[\frac{\partial Q}{\partial\dot{Q}_i}\right]\right|_{\tau=0}=1\ . \tag{C7}$$

We have to take carefully the limit $\epsilon\to 0$ for the "initial conditions" of $D(\tau)$. Note that the matrix of the determinant is only $(N-1)\times(N-1)$ so that we have an extra ϵ to be multiplied. This yields

$$D_1=\frac{2\pi\hbar}{M}\epsilon[2+O(\epsilon)]\to 0 , \tag{C8a}$$

and

$$\frac{D_2-D_1}{\epsilon}=\frac{2\pi\hbar}{M}[3-2+O(\epsilon)]\to\frac{2\pi\hbar}{M} , \tag{C8b}$$

which clearly indicates that

$$D_{N-1}=\left[\frac{2\pi\hbar}{M}\right]\left[\frac{\partial Q}{\partial \dot{Q}_i}\right]\Bigg|_{\tau=t}=\left[\frac{2\pi\hbar}{M}\right]\frac{\partial Q_f}{\partial \dot{Q}_i} . \tag{C9}$$

In fact, a Jacobian is nothing but the density of the paths around the solution of the Langevin equation. This of course agrees with our expectation. The proof for the undamped version can be readily found in textbooks, e.g., Ref. 24. Finally, it should be mentioned that our proof is not restricted to the case of ohmic dissipation.

In general, if there are many particles or the problem is multidimensional, we expect

$$D_{n\text{ particles}}=\prod_{i=1}^{n}\left[\frac{2\pi\hbar}{M_i}\left|\frac{\partial(Q_{1f},Q_{2f},\ldots,Q_{nf})}{\partial(\dot{Q}_{1i},\dot{Q}_{2i},\ldots,\dot{Q}_{ni})}\right|\right] , \tag{C10}$$

although we have not found a simple mathematical proof of this representation (cf. also the comment in Ref. 24). If the system consists of just harmonic oscillators (see Sec. III D) the Jacobian is independent of the paths along which the system "travels," and this is a (time-dependent) constant. In this case, we can obtain (C10) simply from the normalization requirement.

APPENDIX D: UPPER BOUND FOR THE ANHARMONIC EXPANSION

Without loss of generality, let us consider as an example the expectation value of the position given by (2.31) or (6.15). We shall consider the case $\omega_0\neq 0$ (there is no well-defined equilibrium state for $\omega_0=0$). We start with an upper bound of the Green's function $g(\tau)$ [see (6.14)],

$$|g(\tau)|\le a\Theta(\tau)\exp(-b\tau) . \tag{D1}$$

The exact values of a and b are unimportant; for $\eta\to 0$, $b\propto\eta$, whereas for $\eta\to\infty$, $a/b\to$const. Ignoring in (6.16b) the suppression due to the fluctuation, we have

$$|\tilde{S}_n|\le\left|g(t-t_n)\sum_{\{\mu_j=\pm 1\}}\prod_{k=1}^{n-1}R_k\right| , \tag{D2a}$$

where

$$R_k=\frac{1}{\hbar}\sin\left[\frac{\hbar\mu_{k+1}k_0^2}{2}\sum_{l=k+1}^{n}\mu_l g(t_l-t_k)\right] . \tag{D2b}$$

We shall use the following two bounds for R_k (see Maassen[25]):

$$|R_k|\le\frac{1}{\hbar} , \tag{D3a}$$

and

$$|R_k|\le\tilde{R}_k=\frac{ak_0^2}{2}\sum_{l=k+1}^{n}\exp[-b(t_l-t_k)] . \tag{D3b}$$

Turning to the integration over the times $\{t_j\}$, we have

$$\begin{aligned}\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\prod_{k=1}^{n-1}|R_k| &\le\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1 e^{-b(t_2-t_1)}\left[\tilde{R}_2+\frac{a}{2}k_0^2\right]\prod_{k=2}^{n-1}|R_k|\\ &\le\frac{1}{b}\left[\frac{ak_0^2}{2}+\frac{1}{\hbar}\right]\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_3}dt_2\tilde{R}_2\prod_{k=3}^{n-1}|R_k|\\ &\le\cdots\le\text{const}\times\left[\frac{1}{b}\left[\frac{ak_0^2}{2}+\frac{1}{\hbar}\right]\right]^{n-1} .\end{aligned} \tag{D4}$$

This result clearly indicates that (6.15) uniformly converges for sufficiently small V_0. Note that (D3a) is not useful in the classical limit where $\hbar\to 0$. In fact, it might be possible to use only (D1) and (D3b). This yields after some algebra,

$$\begin{aligned}\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\prod_{k=1}^{n-1}|R_k| &\le\int_0^{t_n}dt_{n-1}\cdots\int_0^{t_2}dt_1\prod_{k=1}^{n-1}\tilde{R}_k\\ &\le\left[\frac{ak_0^2}{2b}\right]^{n-1}\left\{\sum_{\{p_l>l\}}^{n}\left[\prod_{j=2}^{n-1}\left[1+\sum_{k=1}^{j-1}\Theta(p_k-j)\right]\right]^{-1}\right\} ,\end{aligned} \tag{D5}$$

where $\Theta(x)$ is the step function [i.e., $\Theta(x)=1$ or 0 for $x>0$ or $x\le 0$] and we sum over all possible configurations: $p_l=l+1,\ldots,n$ and $l=1,\ldots,n-1$. There are $(n-1)!$ terms, but, as one can see, only part of them are important. It is desirable that an efficient bound can be found for the last quantity in (D5).

Finally, we mention that starting directly with the quantum Langevin equation (in operator form), one may obtain a better bound of the series,[26] although one has to be careful in dealing with the quantum operators. Moreover, in the limit $\hbar\to 0$ the series reduces to the solution of the classical Langevin equation, for which a quick bound can be easily found by iteration.

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