Generalized Langevin equation for an oscillator

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A central oscillator coupled to a bath of harmonic oscillators with a two-dimensional Debye spectrum is set up as a model for the dynamics of strongly coupled linear systems. The bath oscillators are eliminated from the central oscillator's equation of motion, other than for initial conditions. The resulting Langevin equation is solved analytically for two different initial conditions for the bath. In one case, the bath oscillators are started at finite temperature and the coupling is turned on suddenly, and in the other they are adiabatically heated with constant coupling. The problem of equipartitioning of the kinetic energy, the velocity autocorrelation function of the central oscillator, and its spectral distribution are examined for various values of the physical parameters. The analytical results of the sudden case are compared with molecular-dynamics calculations and excellent agreement is found.

I. INTRODUCTION

We have recently investigated the dynamics of a damped driven pendulum coupled to a set of harmonic oscillators.[1] The coupling can be choosen so that in one limit (called the strong-coupling limit), the rotor is "free." The precise meaning of the expression was made clear in Ref. 1 and will be discussed again later. The published results based on molecular-dynamics calculations suggested that the system went to thermal equilibrium for the range of parameters considered. However, for some parameter choices there seemed to be a problem with the approach to equilibrium, and certain other questions of principle arose, in particular, how the dynamics behavior depended on initial conditions.

To address the question of the approach to thermal equilibrium and the effect of different initial conditions and values of different physical parameters, we investigate analytically and by molecular dynamics a model in which a central oscillator is coupled to an otherwise uncoupled set of harmonic oscillators, i.e., a completely linear force model. A model of this type was first introduced by Ullersma in a series of papers[2] with a frequency-dependent damping function designed to given an exponential decay law for the central oscillator's autocorrelation functions. This model has recently been examined in a quantum context by Haake and Reinbold[3] (using Ullersma's damping function) and, for our purposes more relevantly, by Wagner.[4] The latter paper shows that the "very definition of the initial state engenders the decay law." This work, however, does not deal with the question of whether this system reaches thermal equilibrium nor does it calculate the spectrum in detail. Our interests are broader. We wish to obtain the spectral representation of the velocity autocorrelation of the central oscillator and to explore whether the system has reached thermal equilibrium or only a steady state. This linear model can serve as a benchmark for the nonlinear case discussed above. Its main advantage is that it can be solved fully analytically and also by molecular dynamics thus allowing one to gauge the accuracy of the numerical technique. The molecular-dynamics results track the analytical ones very well. We hope to return to a fuller analysis of the nonlinear case later with the opportunity of comparing its behavior with the linear-oscillator problem.

II. THE MODEL AND ITS GREEN'S FUNCTION

The model consists of a central one-dimensional (1D) oscillator coupled to a set of oscillators with a two-dimensional (2D) Debye spectrum. The Lagrangian and the equation of motion of the central oscillator are simply linearized versions of those of the rotor model:[1]

$$L=\mu\frac{\dot{\theta}^2}{2}-\frac{\theta^2}{2}+\sum_{i=1}^{N}\left(\tfrac{1}{2}\dot{X}_i^2-\tfrac{1}{2}\Omega_i^2X_i^2+\sqrt{\alpha/N}\,\Omega_iX_i\theta\right) \tag{2.1}$$

and

$$\mu\ddot{\theta}+(1-\alpha)\theta(\tau)+\alpha\int_{\tau_l}^{\tau}H(\tau-\tau')\dot{\theta}(\tau')d\tau'=F(\tau)\ , \tag{2.2}$$

where

$$F(\tau)=\sqrt{\alpha/N}\sum_{i=1}^{N}\{\Omega_iX_i(\tau_l)\cos[\Omega_i(\tau-\tau_l)] +\dot{X}_i(\tau_l)\sin[\Omega_i(\tau-\tau_l)]\}\ . \tag{2.3}$$

The Ω_i in the coupling term ensures vanishing coupling to the zero-frequency modes which normally occurs for

acoustic phonons. We use the initial conditions $\theta(\tau_l)=\dot{\theta}(\tau_l)=0$. All these quantities are in dimensionless units.[1] In the continuum limit ($N\to\infty$)

$$H(\tau)=2\int_0^1 d\Omega\,\Omega\cos(\Omega\tau)\ . \tag{2.4}$$

The Debye oscillator coordinates have been eliminated except for their appearance in $F(\tau)$, the force exerted on the central oscillator, which depends on the initial conditions and uncoupled frequencies of the Debye oscillators. The coupling strength α can vary from zero for an uncoupled central oscillator to unity, where the instantaneous potential vanishes and this oscillator is forced by a term [in addition to $F(\tau)$] dependent only upon the past velocities of the central oscillator itself. We refer to the latter case as the "free"-particle limit. Let us introduce the Green's function g such that

$$\theta(\tau)=\int_{\tau_l}^{\tau} g(\tau-\tau')F(\tau')d\tau'\ . \tag{2.5}$$

Then

$$\dot{\theta}(\tau)=g(0)F(\tau)+\int_{\tau_l}^{\tau}\frac{\partial g(\tau-\tau')}{\partial\tau}F(\tau')d\tau'\ ; \tag{2.6}$$

thus $g(0)=0$ follows from the initial conditions. It will prove useful to introduce the Green's function G by

$$G(\tau-\tau')=\frac{\partial g(\tau-\tau')}{\partial\tau}\ . \tag{2.7}$$

Differentiating Eq. (2.6) again and substituting into Eq. (2.2) leads to

$$G(0)=\frac{1}{\mu}\ , \tag{2.8}$$

and by choosing F to be a δ-function pulse at a time between τ_l and τ gives

$$\mu\frac{\partial^2 g(\tau)}{\partial\tau^2}+(1-\alpha)g(\tau)+\alpha\int_0^{\tau}d\tau'\,H(\tau-\tau')\frac{\partial g(\tau')}{\partial\tau'}=0 \quad \text{for } \tau\geq 0\ . \tag{2.9}$$

The Laplace transform of this equation together with Eq. (2.7) gives

$$\tilde{G}(s)=\frac{s}{s^2[\mu+\alpha\ln(1+1/s^2)]+1-\alpha}\ . \tag{2.10}$$

The Green's function has branch points at $s=\pm i$ and 0. They can be connected by a branch cut running between $\pm i$ along the imaginary axis. The location of the poles of $G(s)$ and its values on the sides of the branch cut are best examined introducing the real variables R and ϕ by

$$Re^{i\phi}=1+1/s^2;\quad R>0,\quad -\pi\leq\phi\leq\pi\ . \tag{2.11}$$

One finds that $\phi=-\pi$ on the edges of the branch cut in the first and third quadrants and $\phi=\pi$ for the remaining two. The pole locations must satisfy the equations

$$\mu+\alpha\ln R_p+(1-\alpha)(R_p\cos\phi_p-1)=0 \tag{2.12}$$

and

$$\alpha\phi_p+(1-\alpha)R_p\sin\phi_p=0\ . \tag{2.13}$$

For $\alpha=0$ (uncoupled central oscillator) Eqs. (2.12) and (13) are solved by

$$R_p=\begin{cases}\mu-1, & \phi_p=\pi, \text{ if } \mu>1\\ 1-\mu, & \phi_p=0, \text{ if } \mu<1,\end{cases} \tag{2.14}$$

$$s_p=\pm i\sqrt{\mu}\ . \tag{2.15}$$

For $0<\alpha\leq 1$, $\phi_p=0$ is a solution of Eq. (2.13), with Eq. (2.12) becoming

$$\mu+\alpha\ln R_p+(1-\alpha)(R_p-1)=0\ . \tag{2.16}$$

The solution for any $\mu>0$ is unique and satisfies $0<R_p<1$. One can show that with $\phi_p\neq 0$ there are no roots consistent with Eq. (2.11). Thus

$$s_p=\pm\frac{i}{(1-R_p)^{1/2}} \tag{2.17}$$

are imaginary and outside of the branch cut except in the limit $\mu=\infty$, when $R_p\to 0$.

The inverse Laplace transform can now be performed on the contour of Fig. 1. There are no contributions from the infinite quarter circles and the contributions of the two contour lines parallel to the negative real axis cancel. The contour surrounding the poles and the branch cut can be pulled tight as a noose. The Green's function can be written as a sum of contributions from the branch cut and the poles

$$G(t)=G_B(t)+G_p(t)\ . \tag{2.18}$$

The contributions from the poles (which are simple poles) is given by

$$G_p(t)=A_p\cos(\omega_p t)\ , \tag{2.19}$$

where

$$A_p=\frac{-1}{1-R_p^{-1}}\frac{1}{\alpha+(1-\alpha)R_p}\ . \tag{2.20}$$

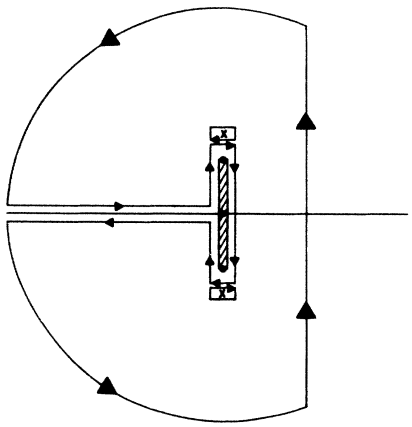

FIG. 1. The contour of integration for the inverse Laplace transform.

R_p is the solution of Eq. (2.16), and the "pole frequency" ω_p is related to R_p by

$$R_p = 1 - 1/\omega_p^2 . \tag{2.21}$$

The contributions from the four sections in the different quadrants of the branch cut can be collected into

$$G_B(t) = \int_0^1 dy\, f(y)\cos(yt) , \tag{2.22}$$

where

$$f(y) = 2\alpha \frac{y^3}{\{-y^2[\mu+\alpha\ln(1/y^2-1)]+1-\alpha\}^2+(\alpha\pi y^2)^2} . \tag{2.23}$$

Note that for $\alpha=1$ the integrand is singular as a function of y but the integral still coverges.

It is instructive to show that Eq. (2.8) is satisfied. In order to perform the integration in Eq. (2.23) for $t=0$ we introduce the transformation

$$y = \frac{1}{(e^z+1)^{1/2}} , \tag{2.24}$$

which we shall repeatedly use in this paper. This leads to

$$G_B(0) = \alpha I_B , \tag{2.25}$$

$$I_B = \int_{-\infty}^{\infty} \frac{dz}{1+e^{-z}} \frac{1}{[\mu+\alpha z-(1-\alpha)(e^z+1)]^2+(\alpha\pi)^2} . \tag{2.26}$$

The poles of the integrand are located at

$$z_n = (2n+1)i\pi, \quad n=0,\pm1,\pm2,\ldots , \tag{2.27}$$

and at the solution ζ_p of

$$\mu+\alpha\zeta_p-(1-\alpha)(e^{\zeta_p}+1)=i\alpha\pi . \tag{2.28}$$

Comparison with Eq. (2.16) shows that

$$R_p = e^{\zeta_p+i\pi} . \tag{2.29}$$

The pole location ζ_p is therefore uniquely related to ω_p by the equation

$$\omega_p = \frac{1}{(1+e^{\zeta_p})^{1/2}} . \tag{2.30}$$

The contribution of the pole at ζ_p to $G_B(0)$ is $-A_p$, canceling precisely the contribution of the pole in $G_p(0)$. The poles at z_n contribute $1/\mu$ to $G(0)$ and Eq. (2.8) is satisfied.

It is useful to introduce the spectral function $A(\omega)$ such that

$$G(t) = \int_0^{\infty} d\omega\, A(\omega)\cos(\omega t), \quad t \geq 0 , \tag{2.31}$$

where

$$A(\omega) = \int_0^1 dy\, f(y)\delta(\omega-y) + A_p\delta(\omega-\omega_p) . \tag{2.32}$$

III. VELOCITY AUTOCORRELATION FUNCTION

The calculation of the velocity autorcorrelation function requires that one calculate

$$\langle\dot\theta(\tau)\dot\theta(\sigma)\rangle = \int_{\tau_l}^{\tau} d\tau' \int_{\tau_l}^{\sigma} d\sigma'\, G(\tau-\tau')G(\sigma-\sigma') \times\langle F(\tau')F(\sigma')\rangle , \tag{3.1}$$

where the lower limit shall be chosen either zero or negative infinity. The force autorcorrelation function is calculated from Eq. (2.3), where again the continuum limit will be taken. Thus

$$\langle F(\tau')F(\sigma')\rangle = \frac{\alpha}{N}\sum_{i=1}^{N}\{\Omega_i^2\langle X_i^2(\tau_l)\rangle\cos[\Omega_i(\tau'-\tau_l)]\cos[\Omega_i(\sigma'-\tau_l)]+\langle\dot X_i^2(\tau_l)\rangle\sin[\Omega_i(\tau'-\tau_l)]\sin[\Omega_i(\sigma'-\tau_l)]\} \tag{3.2}$$

assuming all cross correlations to vanish. Taking the uncoupled Debye oscillators initially in thermal equilibrium at the dimensionless temperature T^*, i.e.,

$$\Omega_i^2\langle X_i^2(\tau_l)\rangle = \langle\dot X_i^2(\tau_l)\rangle = T^* ,$$

we have

$$\langle F(\tau')F(\sigma')\rangle = \alpha T^* H(\tau'-\sigma') , \tag{3.3}$$

where H is defined in Eq. (2.4), and therefore

$$\langle\dot\theta(\tau)\dot\theta(\sigma)\rangle = \alpha T^* \int_{\tau_l}^{\tau} d\tau' \int_{\tau_l}^{\sigma} d\sigma'\, G(\tau-\tau')G(\sigma-\sigma')H(\tau'-\sigma') . \tag{3.4}$$

The temperature dependence is trivial.

We discuss two cases which correspond to two different ways of transferring energy to the central oscillator. In one case, subsection A, we start from $\tau_l=-\infty$ and adiabatically turn on the force $F(\tau)$ and in the other case, subsection B, we turn on $F(\tau)$ suddenly at $\tau_l=0$.

A. Adiabatic turning on of $F(\tau)$

In Kubo's linear-response theory an external force is turned on adiabatically. In the present case this cannot be accomplished by turning on α adiabatically in Eq. (2.3) because α also occurs in Eq. (2.9). The same parameter, the strength of the "external" force, also determines the

spectrum of the system. Thus, turning to Eq. (3.2), instead of turning on α one could supply the Ω_i with identical imaginary parts and incorporate the resulting exponential time dependence into T^* in Eq. (3.2). This situation cannot be physically realized because it amounts to heating the uncoupled Debye oscillators even though they are coupled to the central oscillator. Our excuse for doing so is that the calculation is brief, the result educational, and the comparison with the more realistic case insightful. Formally the exponential time dependence is introduced into the Green's function, rather than into T^*. The time integration can be carried out and one obtains

$$\langle\dot\theta(\tau)\dot\theta(\sigma)\rangle = 2\alpha T^* \int_0^\infty d\gamma \int_0^\infty d\gamma' \int_0^1 d\Omega\, \Omega A(\gamma)A(\gamma') \times \left[\frac{\Omega^2}{(\Omega^2-\gamma^2)(\Omega^2-\gamma'^2)} + \left[\frac{\pi}{2}\right]^2 \delta(\Omega-\gamma)\delta(\Omega-\gamma')\right]\cos[\Omega(\tau-\sigma)] \,. \tag{3.5}$$

There is no oscillation excited at frequencies outside the Debye spectrum. We need to carry out the integral

$$\int_0^\infty d\gamma \frac{A(\gamma)}{\Omega^2-\gamma^2} = \int_0^1 dy \frac{f(y)}{\Omega^2-y^2} + \frac{A_p}{\Omega^2-\omega_p^2} \,. \tag{3.6}$$

The integral on the right-hand side of Eq. (3.6), using the transformation (2.26), becomes

$$\int_0^1 dy \frac{f(y)}{\Omega^2-y^2} = \alpha \int_{-\infty}^{\infty} \frac{dz}{(\Omega^2-1)e^{-z}+\Omega^2} \times \frac{1}{[-(\mu+\alpha z)+(1-\alpha)(e^z+1)]^2+(\alpha\pi)^2} \,. \tag{3.7}$$

Here again ζ_p is a pole but now the infinite set is

$$z_\Omega = \ln\left[\frac{1}{\Omega^2}-1\right] + 2n\pi i, \quad n=0,1,2,\ldots \,. \tag{3.8}$$

Remarkably, the contribution of the pole ζ_p cancels against the last term in Eq. (3.6) and the rather complicated contribution from the poles z_Ω combines with that of the δ functions in Eq. (3.5) to yield

$$\langle\dot\theta(\tau)\dot\theta(\sigma)\rangle = T^* \int_0^1 d\Omega f(\Omega)\cos[\Omega(\tau-\sigma)] \equiv T^* G_B(\tau-\sigma) \,, \tag{3.9}$$

where $f(\Omega)$ is given by Eq. (2.24). Since the result has time translational invariance it is the required autocorrelation function. The integral here is the same one appearing in the branch cut contribution to the Green's function $G_B(t)$. Thus

$$\mu\langle\dot\theta^2(\tau)\rangle = T^*(1-\mu A_p) \,. \tag{3.10}$$

The result shows that the central oscillator does not take on the full equipartition energy unless $A_p=0$. It is only that fraction of the spectrum that overlaps the Debye spectrum that equilibrates, the rest does not get any energy at all. This finding is consistent with the result of Cukier and Mazur,[5,6] according to whom a heavy impurity in a chain comes to equilibrium, but a light one does not.

The difference between this calculation and that of Schwinger[7] is that in his case the bath responded at all frequencies and therefore complete equilibrium was reached. His result for long times corresponds to our adiabatic case. Wagner's results[4] are similar in analytical form to Eq. (3.9), although he uses a different technique, which ignores the possibility of isolated poles and is therefore incomplete. Also he does not pose the question whether the system comes to equilibrium or not.

B. Sudden turning on of $F(\tau)$

In this case the autocorrelation function to be calculated is

$$a(\sigma) = \lim_{T\to\infty} \frac{1}{T}\int_0^T d\tau\langle\dot\theta(\tau)\dot\theta(\tau+\sigma)\rangle \,. \tag{3.11}$$

Here we use σ as a time difference in contrast to the last section. The time integrations are exceedingly tedious. Several terms vanish due to symmetry or in the limit $T\to\infty$. Only two terms survive: One is identical to the first term in Eq. (3.5), the other one requires the evaluation of the integral

$$I = \int_0^\infty d\gamma \frac{A(\gamma)}{\Omega^2-\gamma^2} \int_0^\infty d\gamma' \frac{A(\gamma')}{\Omega^2-\gamma'^2} \frac{\Omega^2+\gamma\gamma'}{2} \times \frac{\sin[(\gamma-\gamma')T]}{(\gamma-\gamma')T}\cos(\gamma'\sigma) \,. \tag{3.12}$$

This integrand involves unusually complicated generalized functions and we are unaware of any rigorous way of evaluating the integral. Our intuitive way of evaluation is justified by the result agreeing with molecular dynamics. In this double integral there are terms originating from the branch cut only, from the poles only, and there are cross terms. The latter ones vanish in the limit $T\to\infty$. The pole contribution includes a factor of the form

$$\sin[(\omega_p-\omega_p)T]/(\omega_p-\omega_p)T$$

TABLE I. The pole frequency and various spectral weights of the central oscillator as functions of μ and α.

μ	α	ω_p	μA_p	P	C	T	MDT
0.5	1	1.59	0.770	0.474	0.229	0.703	0.92
	0.5	1.52	0.836	0.335	0.164	0.499	0.63
	0.1	1.44	0.948	0.108	0.052	0.160	0.20
1	1	1.257	0.582	0.413	0.418	0.831	1.05
	0.5	1.177	0.604	0.335	0.396	0.751	0.89
	0.1	1.067	0.662	0.270	0.337	0.607	0.71
2	1	1.075	0.313	0.264	0.687	0.951	0.96–1.1
	0.5	1.02	0.190	0.168	0.810	0.978	1.04
	0.1	1.00	0.	0.	1.00	1.00	0.96–1.03

which we interpret as a Kronecker δ for $T\to\infty$. The branch cut contribution to the integrand involves the factors

$$\lim_{T\to\infty}\frac{P}{\Omega-y}\frac{P}{\Omega-y'}\frac{\Omega^2+yy'}{2(\Omega+y)(\Omega+y')}\frac{\sin[(y-y')T]}{(y-y')T}$$
$$=\lim_{\epsilon\to 0}\frac{\Omega-y}{(\Omega-y)^2+\epsilon^2}\frac{\Omega-y'}{(\Omega-y')^2+\epsilon^2}\frac{\Omega^2+yy'}{2(\Omega+y)(\Omega+y')}$$
$$\times\frac{\epsilon^2}{(y-y')^2+\epsilon^2}\,, \tag{3.13}$$

where we have interpreted $1/T$ as ϵ, rewritten the principal values using it, and replaced the sine representation of the Dirac δ in the last factor by its Lorentzian representation. The last expression can be regrouped into

$$\lim_{\epsilon\to 0}\frac{\epsilon}{(\Omega-y)^2+\epsilon^2}\frac{\epsilon}{(\Omega-y')^2+\epsilon^2}$$
$$\frac{\Omega^2+yy'}{2(\Omega+y)(\Omega+y')}\frac{(\Omega-y)(\Omega-y')}{(y-y')^2+\epsilon^2} \tag{3.14}$$

which shows that the first two factors alone would become Dirac δ functions in the limit and the third factor would become a number. The last factor decides whether in the limit one really has only the product of two δ functions, of course with the requisite factor $(\pi/2)^2$. Numerical evaluation of the double integral for finite ϵ showed that the last factor can be replaced by unity. Consequently the branch cut term exactly equals the second term of Eq. (3.5) and thus

$$a(\sigma)=\langle\dot\theta(0)\dot\theta(\sigma)\rangle+2\alpha T^*\int_0^1 d\Omega\,\Omega\left[\frac{A_p}{\Omega^2-\omega_p^2}\right]^2\frac{\Omega^2+\omega_p^2}{2}\cos(\omega_p\sigma)\,. \tag{3.15}$$

We conclude that the Fourier transform of the velocity autocorrelation function in the sudden case is the adiabatic result Eq. (3.9) plus a term originating from the pole.

Table I shows for various central oscillator masses (μ) and coupling constants (α), the value of the pole frequency (ω_p), the fraction of the spectral weight at the pole (μA_p), the fractional degree of equipartitioning contributed by the pole (P), by the continuum (C) and the total (T). For $\mu=0.5$ most of the energy is picked up by the central oscillator at the pole, if the interaction is turned on suddenly. For $\mu=2.0$ more energy is picked up in the continuum, and the share of the pole is less or even nearly zero. Note that the spectral weight of the pole decreases as it approaches the Debye frequency with increasing mass. For $\mu=2.0$ and $\alpha=0.1$ the pole has practically merged with the continuum and has no appreciable spectral weight. At this point equipartition is virtually complete. The last column in Table I, MDT, the molecular dynamics result for the fractional degree of equipartitioning is generally appreciably larger than the analytical result. We do not know the reason for this.

IV. ASYMPTOTIC BEHAVIOR OF THE AUTOCORRELATION FUNCTION

The asymptotic behavior of the autocorrelation function depends on whether $F(\tau)$ is turned on adiabatically or suddenly. In the latter case there is an oscillatory contribution at ω_p, absent in the former one. The branch cut contribution can be calculated from Eq. (3.9) for the first case by using a theorem on the asymptotic expansion of Fourier transforms.[8] It shows that the $\Omega\to 0$ behavior of the integrand determines the asymptotic form. The dominant long-time behavior is σ^{-4}, for $0<\alpha<1$. For $\alpha=1$ the integrand diverges as $\Omega\to 0$ and the integral to be evaluated is

$$I(\sigma)=\int_0^1 \frac{d\Omega}{\Omega}\frac{2\cos(\Omega\sigma)}{\left[\mu+\ln\left[\frac{1}{\Omega^2}-1\right]\right]^2+\pi^2}\ .$$

The dominant contribution to the integral comes from Ω near zero both because the cosine oscillates rapidly for large σ and because of the divergence. We estimate

$$I(\sigma)\geq\frac{C}{\ln\sigma},\quad \sigma\to\infty$$

where C is some positive constant. The asymptotic dependence is inverse logarithmic. In the sudden case the conclusions regarding the branch cut contribution are the same. It is important to note that the assumption of a frequency-independent width of the continuum part of the Green's function or of the Fourier transform of the velocity correlation function is not possible in the present case because it is proportional to Ω^2. The frequency renormalization term also depends strongly on Ω [see Eq. (2.23)]. Nevertheless for $\alpha\ll 1$ and $\mu>1$ a Lorentzian line shape is a good approximation in the continuum [see Fig. 2(c)].

V. ASYMPTOTIC BEHAVIOR OF THE KINETIC ENERGY

By performing the integrations in Eq. (3.4) one finds for $\tau_I=0$

$$\langle\dot\theta^2(\tau)\rangle=2\alpha T^*\int_0^1 d\Omega\,\Omega\int_0^\infty d\gamma\frac{A(\gamma)}{\Omega^2-\gamma^2}\int_0^\infty d\gamma'\frac{A(\gamma')}{\Omega^2-\gamma'^2}\{\Omega^2-2\gamma\Omega\sin(\gamma\tau)\sin(\Omega\tau)-2\Omega^2\cos(\gamma\tau)\cos(\Omega\tau)$$
$$+\gamma\gamma'\sin(\gamma\tau)\sin(\gamma'\tau)+\Omega^2\cos(\gamma\tau)\cos(\gamma'\tau)\}\ .$$

In the asymptotic limit there are the following leading terms originating from the several terms in the brackets: constant; periodic at twice the pole frequency; decreasing as $1/\tau^3$ and $1/\tau^4$, and periodic at the pole frequency; and decreasing as $1/\tau^8$.

VI. MOLECULAR DYNAMICS

For the molecular-dynamics calculations we have proceeded similarly to the rotor problem, choosing 100 oscillators to represent the 2D Debye spectrum and solving 101 equations of motion. The equations are the linearized version of those given in Ref. 1, and the technique was fully described there. The results are shown in Fig. 2. Direct comparison of the columns is possible. It can be seen that the molecular-dynamics results are very close to the analytical ones.

Because of the lack of equipartitioning for many values of the parameters in this problem the system generally does not relax to thermal equilibrium. We have therefore tested if a steady state is reached. We found that without any aging at all the results for times corresponding to the first and second 30 Debye cycles are virtually indistinguishable. (A Debye cycle is the time period at the Debye frequency taken as unity.) We therefore always plotted the results for the first 30 cycles. The only exception to this occurs for the parameters $\mu=2.0$ and $\alpha=0.1$, where the second 30 cycles had to be plotted. Apparently for a heavy mass with weak coupling more time is required to pick up energy. The temperature is always taken as unity.

The correspondence with the analytical calculations is excellent, where the curves are smooth. All the peaks within or without the continuum are at the right frequency. In the continuum their heights match. One cannot compare the Dirac δ functions at the poles for the analytic calculations with the peaks of the molecular dynamics which is why they are not shown. Discrepancies also

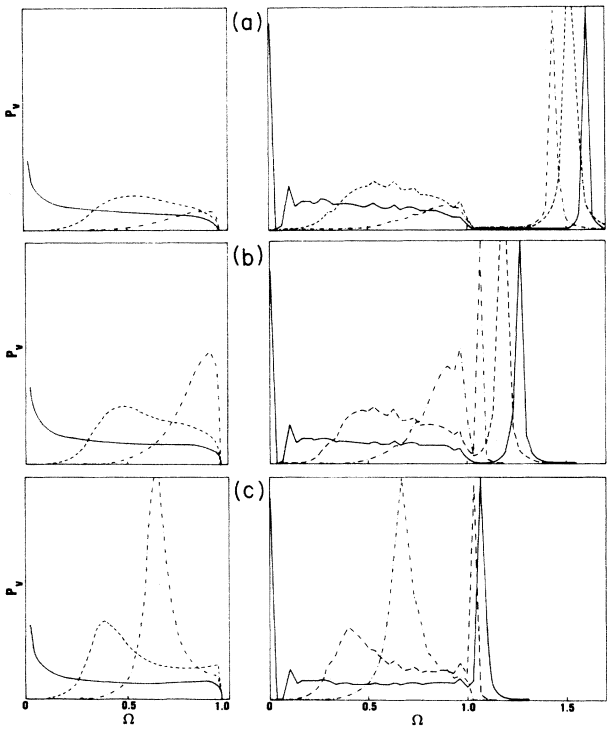

FIG. 2. Spectral function of the velocity autocorrelation function of the central oscillator [$P_v(\Omega)$] in arbitrary units as a function of frequency at $T^*=1$: mass $\mu=0.5$ (a), 1.0 (b), 2.0 (c), for the analytical (column 1) and molecular-dynamics (column 2) calculations; $\alpha=1.0$, ——; $\alpha=0.5$, — — —; $\alpha=0.1$, —·—·—·. Note that for the analytical case we only exhibit the adiabatic results. The sudden calculation adds Dirac δ-function peaks which match the peak positions obtained from molecular dynamics.

occur at the Debye frequency where the molecular dynamics cannot match the discontinuity in the analytic results and, for $\alpha = 1$, at low frequencies. Since the lowest bath oscillator frequency is 0.1 in the molecular-dynamics calculation, where a small peak occurs in the spectrum, the vanishing of the spectral function just below this value is due to the vanishing density of bath oscillators in this regime. The central peak does not diverge because of the finite time run. These results are very encouraging for the continued examination of the rotor case.

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