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Dynamics of a nonlinear oscillator which is coupled to various model heat baths

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We have recently shown that the low-temperature velocity power spectrum of an anharmonic oscillator (AHO) in a canonical ensemble is recovered when one considers the AHO as coupled via harmonic springs to a system of noninteracting harmonic oscillators (HO's), each with the same characteristic frequency as that of the AHO [D.P. Visco, Jr. and S. Sen, Phys. Rev. E **57**, 224 (1998)]. In the present work, we generalize our earlier study by establishing the following points. (i) We show that when the AHO is coupled via anharmonic springs to a system of noninteracting HO's, each with characteristic frequency as that of the AHO, the dynamics of the AHO is strongly affected by the altered coupling and hence we contend that the bath particles must be connected via harmonic springs to preserve the dynamics of the AHO. (ii) We consider an AHO with a characteristic frequency that differs from that of the bath particles and show that the correct dynamics of the new AHO is recovered when (a) the harmonic oscillators that make up the bath particles have constrained movement and (b) the bath particles are harmonically coupled at significantly weakened strength compared to the study in case (i) above. [S1063-651X(98)02508-2]

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I. INTRODUCTION

The study of the dynamics of a single particle in a potential well with the particle being ''weakly coupled'' [1] to a thermodynamically meaningful heat bath is assumed to be correctly described by an analysis done within the framework of a canonical ensemble. Significant literature exists on the time evolution properties of a single *harmonic oscillator* that is in contact with an effective heat bath comprised of many harmonic oscillators [2–4]. One finds that the canonical ensemble dynamics of the harmonic oscillator is correctly obtained if the detailed dynamics of the heat bath is incorporated into the analysis. This article builds upon a previous work [5] and attempts to address the following question: What is the appropriate description of the heat bath when the system consists of a single *anharmonic oscillator* (AHO)?

In a recent work [5], we have shown that various constructs of the heat bath and the coupling between a single particle in an anharmonic potential of the form $V(x)=ax^2+bx^4$ $(ab>0)$ and the heat bath will lead to results that may or may not be consistent with the dynamics predicted by the canonical ensemble. Our conclusion was that a heat bath consisting of noninteracting harmonic oscillators, each in a quadratic well and each being coupled quadratically to the AHO, was one of the appropriate systems for obtaining the predicted canonical ensemble results. In Sec. II below, we summarize the findings of [5] and present some further calculations on the properties of the model bath for the particle in the potential $V(x)=(1/2)x^2+(1/4)x^4$ now with quartic coupling to the bath.

A simple feature of the system described above is that the frequency of the AHO increases monotonically with energy E of the AHO. The lowest characteristic frequency of the AHO is $\omega=1$. In an earlier study, we assumed that the characteristic frequency of the oscillators that make up the heat bath was also unity. We now relax this condition by studying a particle in a potential of the form $V(x)=-(1/2)x^2+(1/4)x^4$, i.e., a particle in a double well potential. In this system, $\omega\to 0$ when E is the barrier height, $\omega\to\sqrt{2}$ when $E\to 0$, and $\omega\to\infty$ as $E\to\infty$. Thus $\omega(E)$ is not a monotonically increasing function of the energy and the lowest frequency of $\sqrt{2}$ is now different from that of the bath oscillators. This work, along with the numerical details of this study, is presented in Sec. III. Section IV contains the concluding remarks and a summary of this work.

II. DYNAMICS OF AN AHO COUPLED TO A HEAT BATH

The Hamiltonian for the particle in an anharmonic potential well, here simply called an anharmonic oscillator, is given by

$$E=p^2/2m+(1/2)x^2+(1/4)x^4, \tag{1}$$

where p and x represent the momentum and position coordinates, respectively, of the anharmonic oscillator and m is the mass of the particle (we set $m=1$ for our analysis here). It has recently been shown through an asymptotic analysis in the canonical ensemble that the relaxation functions (e.g., velocity correlation function and position correlation function) in this system show decay as $1/t$ (t is the beginning time). Additionally, a Fourier transform of this velocity v autocorrelation function (VACF), $\langle v(t)v(0)\rangle/\langle v(0)^2\rangle$, shows a sharp peak in the velocity power spectrum (VPS) at $\omega=1$. This peak, which remains at all temperatures, is dominant only at low temperatures where high-frequency effects are not as strong [6].

In Ref. [5] we have studied the problem of modeling a system that is in thermal contact with a heat bath; the important ideas are how to model the bath itself and how to connect the system to the bath. We chose a single anharmonic oscillator of the form in Eq. (1) above as our system and tried the following constructs to describe the bath, the system, and their coupling.

Model 1 is a bath of harmonic oscillators with nearest-neighbor coupling via harmonic springs. The AHO is connected to each oscillator in the bath by quadratic coupling.

Model 2 is a bath of harmonic oscillators in quadratic potential wells with nearest-neighbor coupling via harmonic springs. The AHO is connected to the bath by quadratic coupling.

Model 3 is a bath of uncoupled (free) harmonic oscillators in quadratic potential wells. The AHO is connected to the bath by quadratic coupling.

It was found that model 3 provided the correct canonical ensemble result ($\omega = 1$) at all ranges of bath size N and system-bath coupling strength K that we tested. Also, an additional high-frequency mode was found that, for large bath size, was proportional to $\sqrt{NK}$. Thus, if this model was used as a bath in a study, this extra frequency could be made to lie outside of the shortest time scales used by the system via a judicious choice of N and K.

To further explore the effects of the type of system-bath coupling, we have modified model 3 to make the coupling between the system and the bath quartic in nature. This model, which we call *model 4*, gives us the Hamiltonian

$$H = p^2/2m + (1/2)x^2 + (1/4)x^4 + \sum_{i=1}^{N} p_i^2/2m_i + \sum_{i=1}^{N} (1/2)(x_i - x_i^0)^2 + K/4 \sum_{i=1}^{N} [x - (x_i - x_i^0)]^4, \quad (2)$$

To reiterate, model 4 is the same as model 3 except the coupling between the AHO and the bath is now with x^4 rather than x^2.

In Eq. (2) above, $m = m_i = 1$ and x_i and p_i are the position and momentum of the ith bath particle, respectively. The AHO is initially placed at the origin. The initial position of bath oscillator i is x_i^0 and is equal to $0.0001i$. A cartoon description of the interactions in all four models is shown in Fig. 1. Before we discuss the results from model 4, a short digression into the numerics of such a study is in order.

A. Simulational details

It is very difficult to solve for the dynamical behavior of the anharmonic oscillator in model 4 in analytic fashion. The equations of motion for each of the particles were therefore solved numerically using the velocity version of the Verlet algorithm [7]. The anharmonic oscillator was assigned an initial velocity of $v = 0.001$.

The velocities of the harmonic oscillators that were used to construct the bath were distributed such that the initial kinetic energy of these oscillators were Boltzmann weighted according to $\exp(-\kappa E_K)$ where E_K is the initial kinetic energy and κ is some constant (we set $\kappa = 1$). The range of kinetic energies allowed was 10^{-4}–25.32. Thus we had equal spacing in $\exp(-\kappa E_K)$ but unequal (i.e., Boltzmann weighted) kinetic energy spacing.

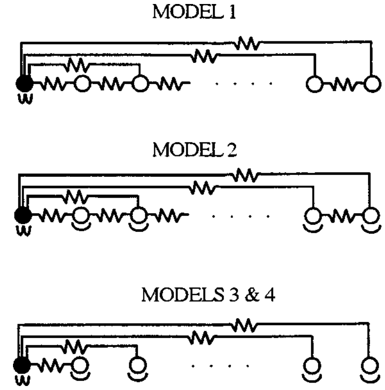

FIG. 1. Cartoon describing the interactions in the four bath models. The filled circle is the particle in the anharmonic well. The open circles are the bath particles. The parabola under some bath particles indicate that those particles are in a harmonic well. The resistors are harmonic (x^2) springs for model 3 and anharmonic (x^4) springs for model 4.

The integration step size and the time length of the study were the same for all sets of N and K studied. The integration time step was 0.000 25 time units. Thus, for 75 000 measurements of the velocity of the AHO, using this time step yields a time length for the study of 18.75 time units.

We have used the discrete cosine transform [8] of the VACF to determine the VPS of the anharmonic oscillator. In order to eliminate the negative numbers that arise from incomplete phase cancellations in the calculation of the discrete cosine transform, we have multiplied the autocorrelation function with a Gaussian function of the form $\exp(-\alpha t^2)$ before taking the transformation. All the velocity power spectra shown in this study have used this Gaussian function with $\alpha = 0.02$.

B. Dynamics of the AHO system in model 4

Before a comparison between the two models could be made, we wanted to verify certain trends in model 4 that were predicted based on the results of our previous study [5], namely, that a large N and a large K will give a velocity power spectrum for the AHO that has the correct canonical ensemble result (i.e., $\omega = 1$) and also that the other contaminants that come in at high frequency do not distort the result at $\omega = 1$. Thus, we conducted six studies at the following set of values for (N,K): $(10,10^{-2})$, $(10,10^{-1})$, $(10,10^{0})$, $(1000,10^{-2})$, $(1000,10^{-1})$, and $(1000,10^{0})$.

The results in the form of the VPS for the AHO are shown in Fig. 2. For the case where $K = 0.01$ [Fig. 2(a)], we see that there is only one peak for a heat bath comprised of ten harmonic oscillators. The contaminants in this state have occurred at such a low frequency that it has distorted the peak predicted by the canonical ensemble at $\omega = 1$. As the bath size is increased to 1000 harmonic oscillators, the peak at $\omega = 1$ is observed as well as two other peaks. The contaminant peak at $\omega \sim 3.4$ is the dominant peak here.

When the coupling is increased by a factor of 10 [Fig. 2(b)], a double peak is seen for the bath comprised of ten harmonic oscillators: one at $\omega = 1.0$ and the dominant peak at $\omega \sim 1.75$. As the bath size is increased to 1000 harmonic oscillators, a dominant peak at $\omega = 1.0$ is observed as well as

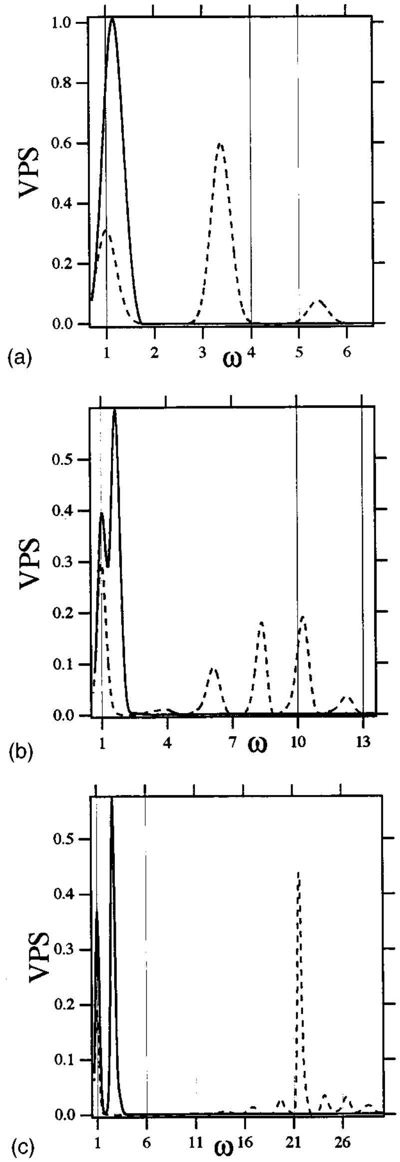

FIG. 2. Velocity power spectrum (arbitrary units) for the anharmonic oscillator connected to the heat bath as described by model 4. The solid line is for the state where $N=10$ and the dashed line for the state where $N=1000$. (a) $K=0.01$, (b) $K=0.1$, and (c) $K=1.0$.

five other peaks at higher frequencies.

At the largest spring constant used, $K=1$, we see [Fig. 2(c)] that two peaks are observed for the ten-harmonic-oscillator bath, but the contaminant peak at $\omega\sim 2.5$ is the dominant one. When 1000 harmonic oscillators are used for the bath several contaminant frequencies are observed in addition to the nondominant peak observed at $\omega=1.0$.

Overall, it is observed for model 4 that as the number of bath oscillators is increased at constant K, the number of contaminants and the frequency at which they occur increase. Additionally, if we look at the case of a constant number of bath particles but increase the coupling constant K, we observe that the frequency at which peaks occur in the velocity power spectrum of the AHO increases.

The next comparison to make is that between model 3 and model 4, namely, which would make a better model of the heat bath and why. To explore this, we obtained the velocity power spectrum for the AHO connected harmonically (i.e., model 3) to a bath of 1000 harmonic oscillators at three different levels of coupling: $K=10^{-2}$, 10^{-1}, and 10^{0}. Since we have already obtained the VPS for the AHO for model 4 at these states, a direct comparison is easily made. Figure 3 shows the VPS of the AHO for both models with $K=0.01$. It is seen that both models have contaminant frequencies in addition to the one at $\omega=1.0$. The quartic coupling has two contaminant frequencies: a dominant one that occurs at a frequency lower than the contaminant for model 3 and a smaller peak at a frequency higher than the model 3 contaminant.

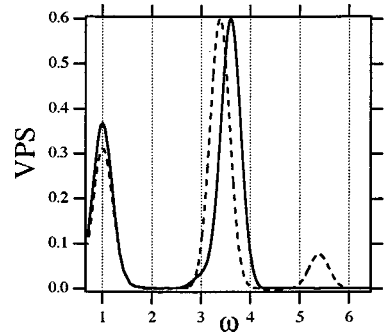

FIG. 3. Velocity power spectrum (arbitrary units) for the anharmonic oscillator connected to the heat bath as described by model 4 (dashed line) and model 3 (solid line) for the state where $K=0.01$ and $N=1000$.

In Fig. 4 we show the VPS of the AHO for both models with $K=0.1$ We see that model 4 has three contaminant peaks at frequencies lower, one peak higher, and one at about the same frequency as the contaminant of model 3.

From Fig. 5, the case where $K=1.0$, we see that all of the contaminant peaks of model 4 occur at frequencies lower than the contaminant of model 3. In fact, the dominant peak of model 4, a contaminant at $\omega\sim 22.0$, has a magnitude that is more than twice as large as that of the peak at $\omega=1.0$. The contaminant of model 3 has about the same magnitude as the peak at $\omega=1.0$.

As mentioned previously, we determined that model 3 has only one contaminant frequency that can be readily predicted at each state of (N,K). For large N, this becomes

$$\omega \propto \sqrt{NK}. \tag{3}$$

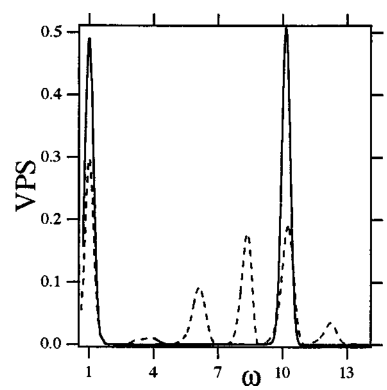

FIG. 4. Velocity power spectrum (arbitrary units) for the anharmonic oscillator connected to the heat bath as described by model 4 (dashed line) and model 3 (solid line) for the state where $K=0.1$ and $N=1000$.

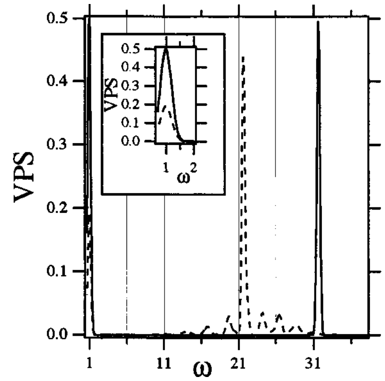

FIG. 5. Velocity power spectrum (arbitrary units) for the anharmonic oscillator connected to the heat bath as described by model 4 (dashed line) and model 3 (solid line) for the state where $K = 1.0$ and $N = 1000$.

On the other hand, it is difficult to predict where or how many contaminant peaks will occur when the coupling between the AHO and the bath is made anharmonic. Clearly, for large N, the trend is that as K increases the contaminants of model 4 are larger in number and lower in frequency than the one contaminant of model 3 as given by Eq. (3). Additionally, the peak at $\omega = 1.0$ for model 4 seems to be decreasing in magnitude as K increases. One may surmise that for some sets of large K and large N, this peak may be totally suppressed for model 4. To investigate this question, we studied the case with $K = 1.0$ and $N = 10\,000$ for both models. As can be seen from Fig. 6, the dominant peak from model 4 is the contaminant that is about 3 times as large as the peak at $\omega = 1.0$. For model 3, the peak at $\omega = 1.0$ is now twice as large as the one contaminant peak at $\omega \sim 100.0$.

Thus it is noted that when studying a system for which the signature frequency in the VPS of the VACF is matched to that of the bath, model 3, relative to model 4, seems to provide the most useful approach to modeling a heat bath for studies on the dynamics of physical systems done within the

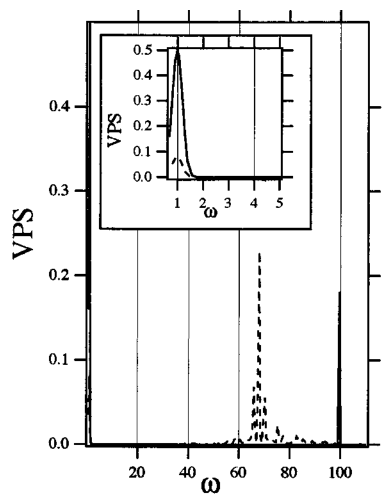

FIG. 6. Velocity power spectrum (arbitrary units) for the anharmonic oscillator connected to the heat bath as described by model 4 (dashed line) and model 3 (solid line) for the state where $K = 1.0$ and $N = 10\,000$. The inset emphasizes the height of the peaks near $\omega = 1.0$.

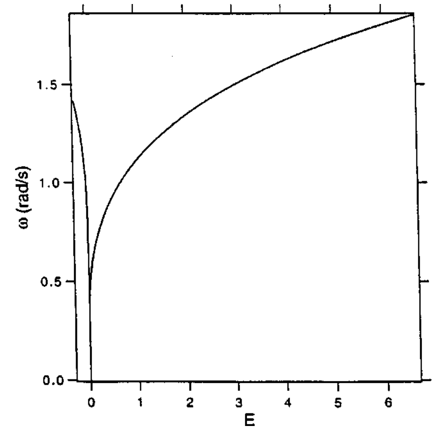

FIG. 7. Frequency of the double well oscillator as a function of its energy.

canonical ensemble. The correct canonical ensemble frequency is obtained at $\omega = 1.0$ and the contaminant frequency can be predicted and be made to lie outside the highest frequencies allowed by the shortest time scales supported by the system of interest. The question now is how well a heat bath described by model 3 will correctly capture the canonical ensemble results of a system that does *not* have its signature frequency matched to that of the bath. This question is explored in the next section.

III. DYNAMICS OF A DOUBLE WELL OSCILLATOR COUPLED TO A HEAT BATH

The Hamiltonian for the particle in a double well potential (DWO) is given by

$$E = p^2/2m - (1/2)x^2 + (1/4)x^4. \tag{4}$$

It is found for this system that the frequency of the DWO does not monotonically increase with the system energy. In fact, there is a nontrivial zero-frequency mode that occurs at an energy equal to that of the barrier height. The frequency of the DWO as a function of energy is shown in Fig. 7.

An analysis very similar to that performed for the AHO was carried out recently [6,9]. Like the AHO, it was found the the VACF in a canonical ensemble decays inversely proportionally to time (a feature that is common to relaxation of particles in anharmonic potentials in which the lowest-order anharmonic term is quartic in nature [6]). The Fourier transform of the VACF showed a sharp peak in the VPS at $\omega = \sqrt{2}$. This peak, which remains at all temperatures, is dominant only at low temperatures where high-frequency effects are weak [6].

The Hamiltonian for the double well oscillator that is harmonically coupled to the bath described by free harmonic oscillators (i.e., model 3) is given by

$$H = p^2/2m - (1/2)(x+1)^2 + (1/4)(x+1)^4 + \sum_{i=1}^{N} p_i^2/2m_i + \sum_{i=1}^{N} (1/2)(x_i - x_i^0)^2 + (K/2)\sum_{i=1}^{N} [x - (x_i - x_i^0)]^2. \tag{5}$$

In an effort to focus on the low-energy dynamics, the DWO is initially placed at the origin, which, according to Eq. (5), is

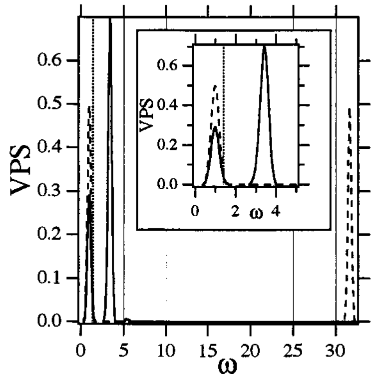

FIG. 8. Velocity power spectrum (arbitrary units) for the double well oscillator connected to the heat bath as described by model 3. The states shown are $N=1000$ and $K=0.01$ (solid line) and $N=1000$ and $K=1.0$ (dashed line). A dotted line shows the canonical ensemble result for the double well oscillator at $\sqrt{2}$.

at the bottom of one of the wells. The initial position of bath oscillator i is x_i^0 and is equal to $0.0001i$.

A. Numerical study of the DWO

The numerical analysis used to examine the dynamics of the DWO in the bath of model 3 is identical to that used for the AHO described in Sec. II A. We will mention specifically in the text to follow where it differs.

B. Dynamics of a DWO using model 3

As before, the goal is to obtain the canonical ensemble frequency for the DWO (i.e., $\omega=\sqrt{2}$) via the model 3 construct of the bath. Figure 8 compares the dynamics of the DWO in the bath of model 3 in terms of the velocity power spectrum for a bath of 1000 particles with two different coupling strengths. It is observed that the signature dynamics of the DWO oscillator in a canonical ensemble is missing ($\omega=\sqrt{2}$) and the frequencies are very similar to that of the AHO in the bath of model 3, namely the peak at $\omega=1$ and the predictable contaminant peak. It was thus thought that the dynamics of the bath characterized by the bath frequency at $\omega=1$, which is now not matched with that of the system at $\omega=\sqrt{2}$, was somehow masking the system dynamics. In an attempt to unmask the system dynamics and make the bath less size dependent, we modified the Hamiltonian of Eq. (5) to make it intensive by dividing all size-dependent terms by N, the number of bath oscillators. (Please note that in all of the studies to follow we have increased the integration step size by a factor of 10, which increases the time length of the study by the same factor. This was done to ensure a sufficient number of periods was completed by the system in calculating the relaxation functions. Such a problem did not arise for the studies involving the AHO.) In Fig. 9 we test the dynamics of the DWO in this new 1000 particle bath by modifying the coupling. The $K=0.01$ system now has an effective coupling of 10^{-5}, while the $K=0.001$ system now has an effective coupling of 10^{-6}. As the effective coupling is lowered, the canonical ensemble frequency for the DWO is recovered, but there is a low-frequency mode that is dominant. It was thought that this low-frequency mode was due to

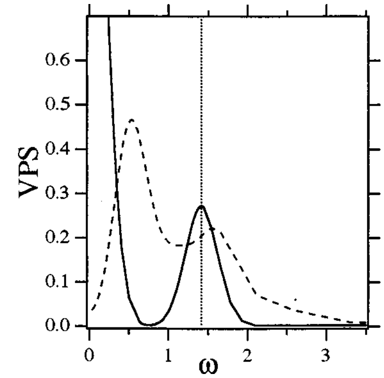

FIG. 9. Velocity power spectrum (arbitrary units) for the double well oscillator connected to the heat bath as described by model 3 with the modification of dividing the extensive terms in the Hamiltonian by N. The states shown are $N=1000$ and $K=0.001$ (solid line) and $N=1000$ and $K=0.01$ (dashed line). A dotted line shows the canonical ensemble result for the double well oscillator at $\sqrt{2}$.

center of mass motion and if this could be removed, an effective description of a bath for the DWO would be attained. Thus we attempted to constrain the motion of the bath particles not with coupling between the bath particles (like models 1 and 2) but by making the quadratic wells in which the bath particles sit much steeper. This constant, which was implied to be equal to unity in the previous models that had this term, now becomes a parameter γ.

C. Refinement of model 3

Thus our Hamiltonian that incorporates the intensivity modification and the well steepness parameter now is

$$\begin{aligned} H=&p^2/2m-(1/2)(x+1)^2+(1/4)(x+1)^4\\ &+(1/N)\sum_{i=1}^{N} p_i^2/2m_i+(\gamma/N)\sum_{i=1}^{N}(1/2)(x_i-x_i^0)^2\\ &+(K/2N)\sum_{i=1}^{N}[x-(x_i-x_i^0)]^2. \end{aligned} \tag{6}$$

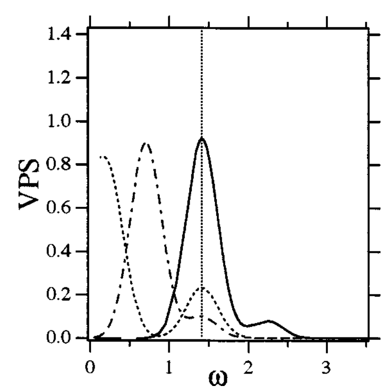

FIG. 10. Velocity power spectrum (arbitrary units) for the double well oscillator connected to the heat bath as described by model 3 with the modification of dividing the extensive terms in the Hamiltonian by N and modifying the bath oscillator wells by a factor of γ. The states shown are $N=1000$ $K=0.001$, and $\gamma=50$ (short-dashed line), $N=1000$, $K=0.001$, and $\gamma=500$ (dot-dashed line), and $N=1000$, $K=0.001$, and $\gamma=5000$ (solid line). A dotted line shows the canonical ensemble result for the double well oscillator at $\sqrt{2}$.

To test this Hamiltonian, we took a bath of 1000 particles with $K = 0.001$ and modified γ over three orders of magnitude. Recall that the VPS in Fig. 9 with $K = 0.001$ has an implied γ equal to unity. The results in terms of the VPS are shown in Fig. 10. When $\gamma = 5000$, we see that the canonical ensemble result is obtained and is the dominant frequency and also the low-frequency center of mass mode has been effectively moved to higher frequencies.

IV. CONCLUDING REMARKS

The details of a many-body system in thermal contact with a heat bath is poorly defined on two fronts. The first question asks what the details of the interactions between the system and bath are. The second question wonders what a heat bath actually is. Even for a few-body system (cluster) and a one-body system, these questions remain. As a first step in a obtaining some understanding of such seemingly complex physics, we have chosen a system comprised of one particle in contact with various models of the heat bath for study. We have determined in this research that the microscopic details of a heat bath can play an important role in affecting the dynamics of a single-particle system with restricted degrees of freedom that is connected to the bath.

For systems whose frequencies are matched to that of the bath, a quadratic coupling between the system and bath is a better bath model than that with quartic coupling. For systems that have characteristic frequencies that are not matched to that of the bath, such as the DWO, modifications to the bath are needed to ensure that the bath does not strongly affect the system and dominate its dynamics. We propose one such model that weakens the coupling by making the bath effects intensive and removes the center of mass modes through restricting the motion of the bath particles. Further study is needed to see if any of these models can be utilized in studies where heat baths are needed to imply constant temperature, such as molecular dynamics simulation in the canonical ensemble.

ACKNOWLEDGMENTS

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