

# Relaxation of classical particles in two-dimensional anharmonic single-well potentials

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(Received 25 August 2000; published 26 January 2001)

The canonical ensemble relaxation function of a particle in a symmetric anharmonic potential well in  $D = 1$  is known to exhibit slow algebraic behavior [S. Sen, R. S. Sinkovits and S. Chakravarti, *Phys. Rev. Lett.* **77**, 4855 (1996); R. S. Sinkovits, S. Sen, J. C. Phillips, and S. Chakravarti, *Phys. Rev. E* **59**, 6497 (1999)]. In the present work, we report a study of relaxation of a particle in symmetric and asymmetric quartic anharmonic potential wells of the form  $V(x,y) = \frac{1}{2}(x^2 + Cy^2) + \frac{1}{4}(x^2 + Cy^2)^2$  in  $D=2$ . The relaxation in the above system is identical to that in  $D=1$  wells when  $C=0$  (since it is then a  $D=1$  system) and  $C=1$ . However, for  $0 < C < 1$  and for  $C \gg 1$ , the frequencies associated with well dynamics are strongly affected and hence the power spectra are altered as a function of  $C$ . Our calculations suggest that the exponents of the long-time tails associated with the relaxation processes are insensitive to  $D$ . In closing, we comment on the consequences of our analysis for the study of slow dynamics in interacting many-particle systems that are connected by harmonic springs with the individual particles in anharmonic potential wells.

DOI: 10.1103/PhysRevE.63.021114

PACS number(s): 05.40.-a, 65.90.+i

## I. INTRODUCTION

The study of relaxation processes in disordered lattices remains a problem of fundamental interest in the physics of glassy systems [1,2]. An essential difficulty encountered in studying the dynamics of these systems concerns the limitations in our ability to study relaxation processes of these systems across many decades in time [3]. Such limitations force us to make assumptions about ergodicity and nonergodicity of these systems [4]. These assumptions typically remain unproven. The available theories of glassy relaxation are therefore purely phenomenological, leaving significant voids in our understanding of the microscopic dynamical processes in these systems and in our ability to predict and control the properties of glassy systems [5].

In the present study, we build on earlier work to address the problem of nonlinear dynamics at fixed energies and of canonical ensemble relaxation functions at fixed temperature in single anharmonic wells in  $D=2$ . We refer to arguments presented in detail in Refs. [6],[7], which imply that such a study might be relevant to the development of a microscopic understanding of the long-time relaxation processes encountered in studying the dynamics of disordered interacting systems.

This article is arranged as follows. In Sec. II, we present the model system and outline the method of study. In Sec. III we present the canonical ensemble results for the symmetric two-dimensional (2D) system. In Sec. IV we probe the more difficult asymmetric quartic well potential that can be characterized by a parameter  $C$  (defined below) taking values between 0 and  $\infty$ . We find linearity in the directional frequencies as a function of energy as we approach zero energy, which in turn allows us to infer the long-time tail in the canonical ensemble relaxation function [9], in a  $D=2$  asymmetric single-quartic-well potential. The study is summa-

rized in Sec. V with comments on the possible future of our efforts.

## II. THE MODEL AND ITS ANALYSIS

We begin by considering a system defined by the potential

$$V(x,y) = \frac{A}{2}(x^2 + Cy^2) + \frac{B}{4}(x^2 + Cy^2)^2 \quad (1)$$

whose behavior is controlled by the parameters  $(A,B,C)$ . In the present study we take  $A=B=1$ . (We remind the reader that  $A=-1$  leads to a double-well potential, which we do not address in this work [6,7,9].) The parameter  $C$  controls the symmetry of the potential surface.  $C=0$  and 1 yield a  $D=1$  system and the planar-symmetric  $D=2$  system, respectively. The other values of  $C$  yield a  $D=2$  surface with planar asymmetry. As we shall see,  $C=0$  and 1 lead to relaxation behavior observed in  $D=1$ . Interesting behavior arises when  $C \neq 1$ . This case is discussed in Sec. IV.

The equations of motion for this system are

$$\ddot{x} = -Ax - Bx^3 - BCxy^2, \quad (2)$$

$$\ddot{y} = -ACy - C^2By^3 - BCx^2y, \quad (3)$$

and represent an unsolved set of equations whose solution is numerically constructed using the velocity version of the Verlet algorithm, with step size of 0.01 time units. Note that all values in this and subsequent equations are dimensionless. Observe that for  $C=0$  Eqs. (2) and (3) reduce to the well known equation for the Duffing oscillator [8]. The dynamics of the Duffing oscillator was solved back in 1918. Relaxation in Duffing potentials has been reported in [6,7,9].

### A. Symmetric potentials

In a previous study [6,7] for symmetric potentials, it was shown that the relaxation behavior at fixed temperatures, i.e., in canonical ensembles, is obtained by performing a Boltzmann weighted sum of relaxation functions at *fixed energies* (i.e., in the context of a microcanonical ensemble context). The normalized relaxation function of some dynamical variable  $\Psi(t, E)$  in the canonical ensemble is then given by an energy integration over various levels of the microcanonical ensemble relaxation function,

$$\begin{aligned} & \left\langle \frac{\Psi(t)\Psi(0)}{\Psi^2(0)} \right\rangle_{\beta} \\ &= \frac{\int \int_{E, t'} \Psi(t', E) \Psi(t'+t, E) g(E) \exp(-\beta E) dt' dE}{\int \int_{E, t'} \Psi^2(t', E) g(E) \exp(-\beta E) dt' dE}, \end{aligned} \quad (4)$$

where  $g(E)$  denotes the density of states. The reader may note that  $g(E)$  is a constant at low enough energies and can be incorporated into an analysis where uneven step sizes are used in the energy integration to account for peaks in  $g(E)$  across some energy range [6,7,9].

For this study,  $\Psi(t, E)$  is chosen to be the velocity and  $\beta=1$ . Thus, we consider the behavior of the velocity autocorrelation function (VACF). The choice of  $\beta=1$  does not restrict the conclusion of this study regarding long-time tails, which, as we show later, turn out to be temperature independent. The integration was performed using 5000 energy levels whose values ranged from near 0 (the well minimum) to  $E \sim 25$ . Note that in the calculation using Eq. (4) first the microcanonical relaxation function is determined at all the energy levels by determining the dot product of the velocity (in a chosen direction) at some reference time ( $t'$ ) with that of the velocity (in the same direction) at some later time ( $t'+t$ ). This quantity is summed over many periods and normalized to provide the microcanonical relaxation function at that energy level.

### B. Asymmetric potentials

A convenient feature of the symmetric potential studied is the ability to extract long-time information on a constant energy system through use of the period of the motion of the system. However, when  $C \neq 1$ , this symmetry does not exist and it is hence necessary, through many time steps, to ascertain the position and velocity of the system directly at long times. Since the autocorrelation functions of many energy levels are required for this study, the method used previously for the symmetric potentials is precluded.

However, as proved in recent work by Sarkar [9], if we can establish that the frequency  $\omega \propto E$  as  $E \rightarrow 0$ , this implies a decay of  $1/t$  for the velocity autocorrelation function in a canonical ensemble. Thus, we attempt to find this relationship in order to establish a  $1/t$  decay for these asymmetric wells.

As an aside for readers whose knowledge of autocorrelation function decay is limited to exponentials, we provide the

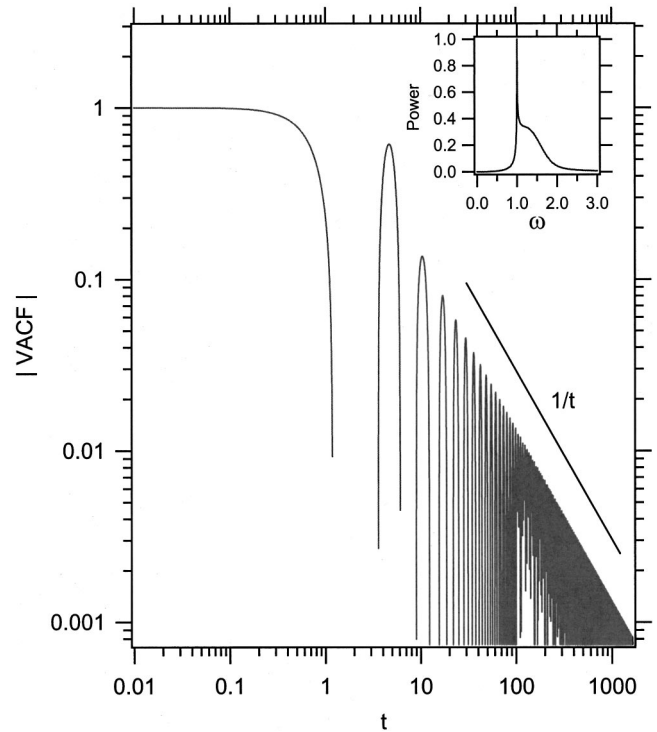


FIG. 1. Plot of the absolute value of the VACF versus time for a particle in a symmetric quartic potential characterized by  $C=1$ . The long-time relaxation is  $1/t$  in nature. Note that the power spectrum in the inset is given in arbitrary units.

following paragraph. In cases where relaxation behavior exhibits exponential-like decay, one typically finds a combination of very fast time-scale dynamics and relatively slow time-scale dynamics. Examples are (i) the intermediate time relaxation of a massive object in a system of light oscillators [10]; (ii) relaxation of an impurity in an  $s = \frac{1}{2}$  XY chain [11]. In the case of relaxation of a particle in a 2D anharmonic well, there are no obviously disparate time scales. Hence, one would not expect exponential relaxation to equilibrium but rather a decay in which characteristic time scales are absent, such as an algebraic decay. It is noteworthy that the  $1/t$  decay found in 2D systems is the same as that in 1D systems and that removal of system symmetry leaves the asymptotic relaxation behavior invariant.

### III. SYMMETRIC POTENTIAL: RESULTS

For the symmetric ( $C=1$ ) system, analysis is facilitated by analyzing the  $x$  and  $y$  directions separately. However, the period of motion of the system is the same for a given energy in both directions which leads to the same microcanonical autocorrelation functions. Thus, the canonical autocorrelation function and corresponding power spectrum will be invariant of the direction studied. Hence we will work in only the  $x$  direction knowing that the  $y$  direction will be identical. Figure 1 shows the velocity autocorrelation function and corresponding power spectrum for this symmetric potential. A regression on the peak heights of the VACF as a function of time yields a decay  $\sim 1/t$ , as shown in Fig. 1. The results

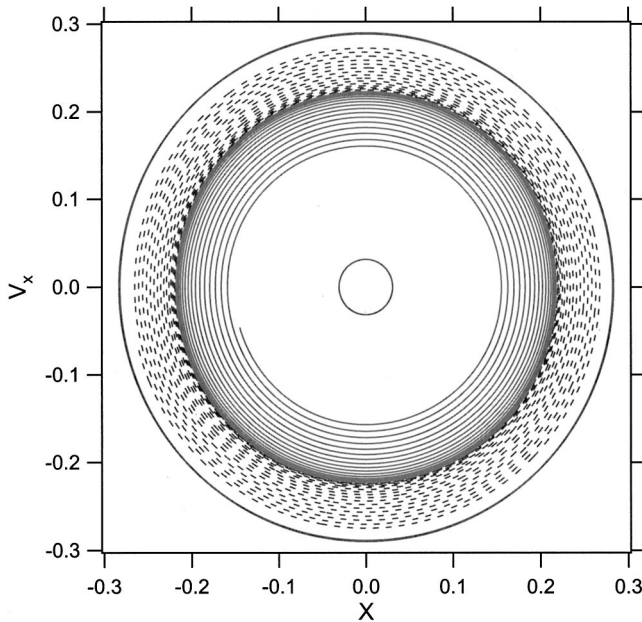


FIG. 2. Plot of  $x$  component of velocity of the particle,  $v_x$ , as a function of position  $x$  for various values of the symmetry parameter  $C$  at  $E=0.05$  (see extended discussion in Sec. IV).

agree completely with the relaxation behavior reported in the 1D studies in Refs. [6], [7].

#### IV. ASYMMETRIC POTENTIAL: RESULTS

The goal here, once again, is to ascertain whether we can express the lowest frequencies as a linear function of the energy, as we approach the well minimum (i.e., as  $E \rightarrow 0$ ). Since the potential energy is now asymmetric, we need to specify the direction; thus we will study both the  $x$  and  $y$  directions separately. After sufficient study, it was determined that exploring energies between  $10^{-1}$  and  $10^{-2}$  would enable us to expose the behavior we wished to study.

For the energy range tested, we performed simulations using various values of the parameter  $C$ . For very small values of  $C$  the potential becomes very nearly a 1D problem (in the  $x$  direction), but clearly the cross terms in Eqs. (2) and (3) become less important, making this almost two separate 1D problems, one in  $x$  and the other in  $y$ . That this is true is seen in the phase space plots for both directions, given in Figs. 2 ( $x$  direction) and 3 ( $y$  direction) for 100 time units at an energy of 0.05. In Fig. 2, the outermost circuit is for  $C=0.2$  and the effect of the  $y$  direction coupling is negligible. Likewise, in Fig. 3 the horizontal oval is for  $C=0.2$  and there is negligible  $x$  direction coupling in the  $y$  direction. As  $C$  increases toward 1, the cross terms in Eqs. (2) and (3) are of the same order of magnitude as the diagonal terms and the effects of the coupling are seen very clearly in the phase space plots. In Fig. 2, the dashed line that is spiraling away from the center is for  $C=0.99$ . Figure 3 shows this same effect in the  $y$  direction; this time the dashed line spirals toward the center. At  $C=1.0$ , we recover the symmetric case and, accordingly, the phase space plots are exactly circles for both the  $x$  and  $y$  directions. At  $C$  slightly greater than unity,

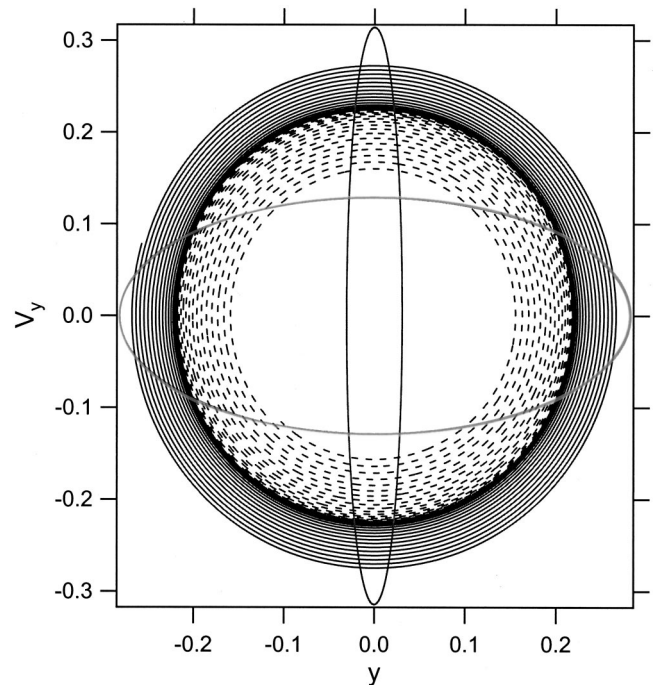


FIG. 3. Plot of  $y$  component of velocity of the particle,  $v_y$ , as a function of position  $y$  for various values of the symmetry parameter  $C$  at  $E=0.05$  (see extended discussion in Sec. IV).

we once again lose symmetry. Figure 2 shows the states for  $C=1.01$ , a solid line spiraling in toward the center. Likewise, the  $y$  direction for this state shows a solid line spiraling away from the center. For very large values of  $C$ , the problem once again approaches a one-dimensional problem, this time in the  $y$  direction. The  $C=100$  case is shown in Fig. 2 as the small circle in the center while Fig. 3 shows the  $y$  direction, which is a vertical oval.

In order to determine if the frequency is linear in energy

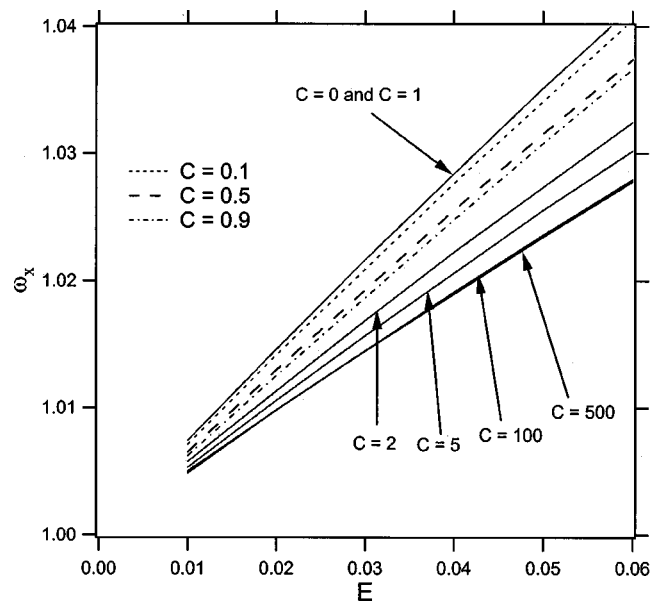


FIG. 4. Plot of  $\omega_x$  versus  $E$  for  $500 \geq C \geq 0$  showing that  $\omega_x \propto E$  as  $E \rightarrow 0$ .

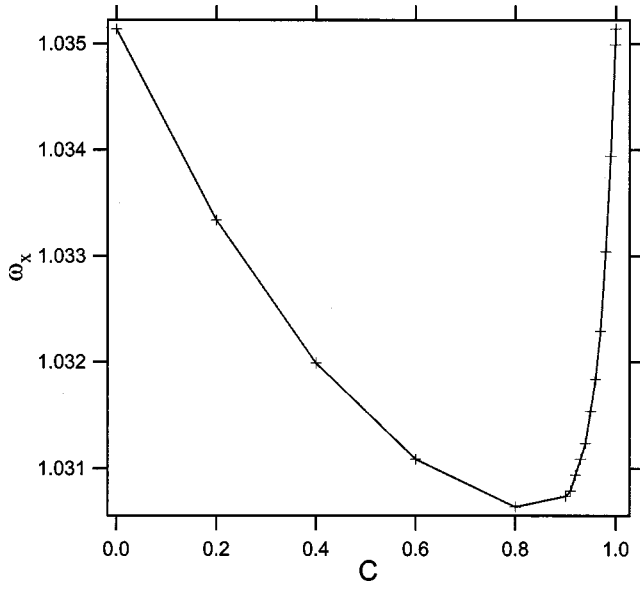


FIG. 5. Plot of  $\omega_x$  versus  $C$  for  $E=0.05$ . Observe that  $\omega_x$  is the same for  $C=0$  and 1. The systems begins to become sharply 1D-like for  $C \sim 0.9$ .

and thus make a statement about the decay rate of the VACF in the canonical ensemble of this potential, we explore the frequency in each direction (both  $x$  and  $y$ ) as a function of  $C$  and  $E$ .

#### A. $x$ direction

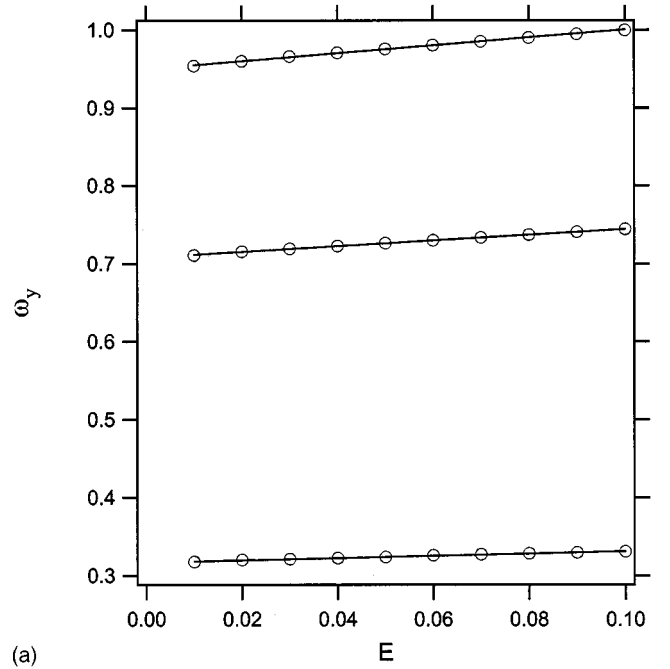
In Fig. 4 we show the  $x$  direction frequency as a function of energy for various values of  $C$ . It is clear from Fig. 4 that there is a linear dependence of frequency as a function of energy for small enough energies. It is interesting, however, to note what occurs when  $C$  takes on values between 0 and 1. Recall that the  $C=0$  state is a 1D problem, while the  $C=1$  state is the symmetric 2D problem. Both of these symmetric systems should provide the same  $x$  direction frequency and this is seen in Fig. 4. When we look at how the  $x$  direction frequency changes with  $C$  at a constant energy, we find the function to be unimodal in that range, with each end point giving the same frequency. This is shown in Fig. 5 for the state where  $E=0.05$ .

#### B. $y$ direction

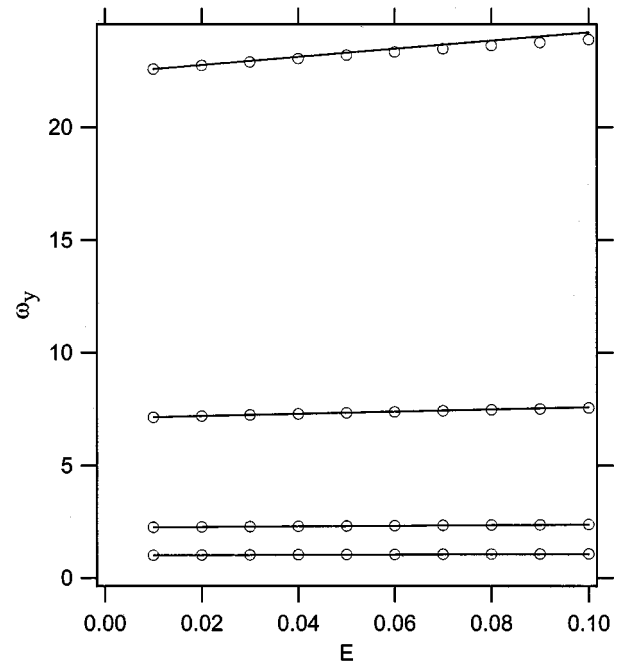
In Fig. 6 we show the  $y$  direction frequency as a function of energy for various values of  $C$ , both less than and greater than unity [Figs. 6(a) and (b)]. It is clear from these figures that there is a linear dependence of this frequency on the energy of the system at low energy. However, it is of interest to see if fitting parameters for this linear form can be given as a function of  $C$ , thus reducing all the data shown in Fig. 6 into one function of  $E$  and  $C$ . The form is reported as

$$\omega_y(E, C) \approx \sqrt{C} + (0.536C^{0.567})E, \quad (5)$$

and the quality of fit is demonstrated by the lines in Figs. 6(a) and 6(b).



(a)



(b)

FIG. 6. Plot of  $\omega_y$  versus  $E$  for various values of the symmetry parameter  $C$ . In (a), the values plotted (reading from top to bottom) are  $C=0.9, 0.5$ , and  $0.1$ ; in (b),  $C=500, 50, 5$ , and  $1$ .

With both the  $x$  and  $y$  directions having a linear dependence on the frequency as a function of energy as energy  $\sim 0$ , we can, via the work of Sarkar [9], conclude that the decay of the VACF for these asymmetric potentials in the canonical ensemble will be  $1/t$ .

## V. CONCLUSIONS

In this article we have demonstrated via extensive numerical studies that the long-time tail of the VACF of a particle



in an asymmetric 2D single-well quartic potential behaves as  $1/t$ . This long-time tail turns out to be the same as that found in 1D quartic wells and is possibly independent of the spatial dimension of the system, a result that would have been difficult to establish without careful numerical analysis. The present result, along with the arguments in Sec. VII of Ref. [6] [see Eqs. (45)–(50)], suggests that slow relaxation in local wells will dominate the low temperature relaxation in glassy systems that can be generically modeled via particles

connected via harmonic springs and with on-site anharmonic potentials [12].

#### ACKNOWLEDGMENTS

We acknowledge helpful discussions with Professor D. C. Mattis, Professor Raj K. Pathria, Professor Subir K. Sarkar, Professor Deepak Dhar, Professor S. D. Mahanti, and Professor M. Howard Lee. The research was partially supported by the National Science Foundation and by Sandia National Laboratories.

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