Algebraic relaxation of classical particles in one-dimensional anharmonic potentials: Analytical proof

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We prove that for the one-dimensional motion of a classical particle in a potential of the form $V(x)=ax^2+bx^{2n}$ with $a,b>0$ and n equal to a positive integer greater than or equal to 2, the thermally averaged velocity autocorrelation function $C(t)$ behaves as a sinusoidal function of time divided by $t^{1/(n-1)}$ as t goes to infinity. This form of the correlation function survives some alterations in $V(x)$, which we discuss. [S1063-651X(96)06709-8]

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Investigation of the relaxation properties of a classical particle in a one-dimensional anharmonic potential is a problem of considerable general interest because of its connection to a variety of problems in condensed matter physics, e.g., thermally activated dynamics in glass transitions or the Krumhansl-Schrieffer model of structural phase transition [1–6]. Recently, Sen, Sinkovits, and Chakravarti studied such dynamics for potentials of the form $V(x)=ax^2+bx^{2n}$ with $a,b>0$ and $n=2$, 3, 4, and 5 [7,8]. For $n=2$, they showed (both numerically and analytically) that the thermally averaged velocity autocorrelation function $C(t;\beta)$ decays asymptotically as $1/t$ apart from an overall periodic prefactor. Here $\beta=1/k_BT$ where T is the temperature. For $n=3$, 4, and 5 their numerical work suggests that the asymptotic decay is again algebraic and with an exponent equal to $1/(n-1)$. In this work we prove analytically that their results are quite generally valid. To be precise, we prove that $C(t;\beta)$ asymptotically goes as $P(t)/t^{1/(n-1)}$ where n is any positive integer greater than or equal to 2 and $P(t)$ is a sinusoidal function of time with the periodicity the same as that associated with the motion when the energy goes to zero. This form of the correlation function as a product of a sinusoidal function and an algebraic function survives even if a is negative or linear and cubic terms are added to the potential. Thus we have provided analytical support to all the numerical results of Ref. [8] and have generalized the results considerably.

To derive these results, first we take the case when the potential is of the form $V(x)=(1/2)x^2+(1/2n)x^{2n}$, where n is a positive integer greater than or equal to 2. The definition of the thermally averaged velocity autocorrelation function is

$$C(t;\beta)=\left(\int_0^\infty \exp(-\beta E)d(E)h(t;E)dE\right)\Big/\left(\int_0^\infty \exp(-\beta E)d(E)dE\right), \tag{1}$$

where $d(E)$ is the density of states and $h(t;E)$ is the autocorrelation function at energy E. Since the motion with a particular energy E is bounded and periodic with frequency $w(E)$, $h(t;E)$ is also periodic with the same frequency. The definition of $h(t;E)$ is

$$h(t;E)=\left(\int_{-\infty}^{\infty} v(t')v(t+t')dt'\right)\Big/\left(\int_{-\infty}^{\infty} v(t')^2dt'\right). \tag{2}$$

Since the velocity is a periodic function of time, it can be written in the form

$$v(t)=\sum_{p=0}^{\infty} a_p(E)\sin[(2p+1)w(E)t]. \tag{3}$$

The fact that there are no cosine terms in this expansion is simply a consequence of the choice of phase. The origin of the time axis is taken to coincide with a moment when the particle is at one of the two turning points of motion. Only odd multiples of the fundamental frequency appear in the series since $V(-x)=V(x)$. Thus substituting (3) in (2),

$$h(t;E)=\left(\sum_0^\infty a_p^2(E)\cos[(2p+1)w(E)t]\right)\Big/\left(\sum_0^\infty a_p^2(E)\right). \tag{4}$$

The denominator of the right-hand side of Eq. (4) is nothing but the action $J(E)$ of the orbit defined by $J(E)=\oint p(x)\,dx$ with a mass of 1. So Eq. (4) reduces to

$$h(t;E)=\left(\sum_0^\infty a_p^2(E)\cos[(2p+1)w(E)t]\right)\Big/ J(E). \tag{5}$$

Since our basic goal is to study the time dependence of the correlation function, we are not concerned with the denominator in Eq. (1) and shall study only the function

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$$G(t;\beta)=\int_0^\infty \exp(-\beta E)d(E)h(t;E)dE \tag{6}$$

$$=\int_0^\infty dE\ \exp(-\beta E)\times d(E)\sum_{p=0}^{\infty}[a_p^2(E)/J(E)]\times\cos[(2p+1)w(E)t]. \tag{7}$$

Let us take the pth term $[G_p(t;\beta)]$ of this series and find out its asymptotic behavior. $G_p(t;\beta)$ is the real part of I_p, where

$$I_p=\int_0^\infty dE\ \exp(-\beta E)d(E)[a_p^2(E)/J(E)]\times\exp[it(2p+1)w(E)]. \tag{8}$$

I_p has the form $\int_a^b f(E)\exp[it\phi(E)]dE$ with both f and ϕ real, $a=0$ and $b=\infty$ and we are interested in the $t\to\infty$ limit. We apply the well-known method of stationary phases [9] to accomplish this goal. The crucial element of our analysis is to note, without any proof for the time being, that $\phi(E)$ has a $(n-1)$th order stationary point at $E=a=0$. This means that all the derivatives of $w(E)$ up to and including the $(n-2)$th order vanish at $E=0$ but the $(n-1)$th order derivative is nonvanishing.

Let us first take the $p=0$ term, which will turn out to be the term decaying the slowest and hence give the leading asymptotic behavior. As E goes to zero, $d(E)$ approaches a nonzero constant. To see this note that the number of states $[N(E)]$ with energy up to E is proportional to the area in the x-p plane enclosed by the contour of energy E. As E goes to zero, the motion becomes essentially harmonic and this area is proportional to E. Similarly, a_0^2 is also linear in E so that $a_0^2/J(E)$ approaches a nonzero constant. This statement is again a consequence of the observation that in the $E\to0$ limit, the motion is harmonic to leading order. Thus $f(E)$ goes to a nonzero limit as $E\to0$. As $t\to\infty$, the leading behavior of I_0 is then given by [9]

$$I_0(t)\sim f(0)\exp[it\phi(0)+i\pi/2m][m!/t|\phi^{(m)}(0)|]^{1/m}\times\Gamma(1/m)/m, \tag{9}$$

where $m=(n-1)$ and $\phi^{(m)}(0)$ is the mth derivative of ϕ evaluated at $E=0$. Since $G_0(t;\beta)$ is the real part of $I_0(t)$, it immediately follows that, in general

$$G_0(t;\beta)\sim\cos[w(0)t+\pi/2(n-1)]/t^{1/(n-1)}. \tag{10}$$

This is the basic result we wanted to prove. For values of p higher than zero, $a_p^2(E)$ involves powers of E higher than one. The actual powers will depend on the specific choice of potential. Thus $f(E)$ goes as $E^{l(p)}$ in the $E\to0$ limit. Here l is a strictly increasing function of p. It is simple to see [9] that in such a situation I_p will have additional powers of t in the denominator and thus decay faster than I_0. Higher values of p will thus contribute progressively faster decaying terms to the correlation function.

The statement that $w(E)$ has an $(n-1)$th order stationary point at $E=0$ follows from results available in the work of Codaccioni and Caboz [10] where the dependence of time period on energy is shown to be a generalized hypergeometric function of $E^{(n-1)}$. This implies that in the limit $E\to0$, $w(E)$ has the form of $w(E)=w(0)+\text{constant}\ E^{(n-1)}$. In the following we will give an alternative proof of this result. The proof depends on the fact that $1/w(E)=dJ(E)/dE$. Thus we need to show that $J(E)=\alpha_1E+\alpha_2E^n+$ (higher order terms). Now, since the potential is symmetric around $x=0$,

$$J(E)=4\int_0^{U(E)}\sqrt{2\{E-(1/2)x^2-(1/2n)x^{2n}\}}dx, \tag{11}$$

where $U(E)$ is the right turning point. In Eq. (11) the integral without the anharmonic term [the right turning point then being $U_0(E)=\sqrt{2E}$] is α_1E. Thus we need to show that the leading term in $\delta J=\int_0^{U_0(E)}\sqrt{E-(1/2)x^2}dx-\int_0^{U(E)}\sqrt{E-(1/2)x^2-(1/2n)x^{2n}}dx$ is of order E^n:

$$\delta J=\int_0^{U(E)}[\sqrt{E-(1/2)x^2}-\sqrt{E-(1/2)x^2-(1/2n)x^{2n}}]dx+\int_{U(E)}^{U_0(E)}\sqrt{E-(1/2)x^2}dx=T_1(E)+T_2(E). \tag{12}$$

$U(E)$ can be determined easily through perturbative techniques [9] and is given by

$$U(E)=\sqrt{2E}-(1/2n)(2E)^{(2n-1)/2}+\{[2n-(1/2)]/4n^2\}(2E)^{2n-(3/2)}+\cdots. \tag{13}$$

Using this it is straightforward to see that $T_2(E)\sim E^{(3n-1)/2}$. To calculate $T_1(E)$ notice that $\{\sqrt{E-(1/2)x^2}-\sqrt{E-(1/2)x^2-(1/2n)x^{2n}}\}=[(x^{2n}/2n)/\sqrt{E-(1/2)x^2}]f(x)$, where $f(x)=[1-\sqrt{1-y(x)}]/y(x)$ with $y(x)=(x^{2n}/2n)/[E-(1/2)x^2]$. The range of x $[0,U(E)]$ maps onto the range $[0,1]$ for y and thus $f(x)$ is bounded above by 1 and below by σ with $1>\sigma>0$. The important point here is that σ is independent of E. Thus $T_1(E)$ is bounded above and below by K and σK, respectively, where $K=\int_0^{U(E)}\times(x^{2n}/2n)/\sqrt{E-(1/2)x^2}dx$ and is easily shown to be of the order E^n. Since $T_1(E)$ is bounded both above and below by quantities of order E^n in the limit $E\to0$ it must be strictly of order E^n in this limit and thus dominates T_2 (since n is greater than or equal to 2). Thus δJ is of order E^n. This completes the proof.

In the potential $V(x)=ax^2+bx^{2n}$, which we have been considering until now, both a and b were taken to be positive. We can generalize our results to the situation when a is negative and when, in addition, linear and cubic terms are added to the potential. If $a<0$ the potential assumes a double well shape whereas addition of linear and cubic terms makes the potential asymmetric. In these situations the global potential minimum (or minima) shifts away from $x=0$. When the potential is expanded in terms of displacement from such a minimum, the first term is quadratic with positive coefficient and this is followed by a cubic term. The degree of the polynomial of course remains unaltered. Remember that the object of primary interest to us is the leading correction to the constant term in the expression for $w(E)$. Again, we use the result from Ref. [10] that when the first correction to the harmonic potential is cubic, the leading correction in $w(E)$ is linear in E. Thus again the algebraic part of $C(t)$ is $1/t$. $w(0)$ has to be computed keeping in mind that the potential minimum has shifted away from $x=0$. The analytical results presented in this paper completely explain all the numerical results described in Ref. [8].

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