



A STUDY OF CURRENT CORRELATION FOR OSCILLATORS WITH CUBIC AND QUARTIC ANHARMONICITIES

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ABSTRACT

A detailed investigation for the wave number and time dependence of the classical current correlation function (CCF) for the oscillators with cubic and quartic anharmonicities has been carried out. This goal has been achieved by identifying a reference harmonic oscillator (HO) such that the difference between its Helmholtz free energy from that of the actual anharmonic oscillator (AHO) up to first order in thermodynamic perturbation theory for a specific temperature is the minimum. This minimization is performed by treating the eigenfrequency of the HO and the shift in the point of the minimum in its potential energy w.r.t. that of the relevant AHO as two variational parameters. The eigenfrequencies so obtained have, in turn, been used to determine the CCF through the exact formula recently derived by Wierling and Swada. Also included are the results for rate of variation of CCF with wavenumber and time.

I. INTRODUCTION

Amongst the variety of time correlation functions, the current correlation function (CCF), defined as

$$CCF = \langle J_k^*(t) J_k(0) \rangle = \frac{1}{Z} \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dp e^{-\beta H} p(t) e^{-ikq(t)} p(0) e^{ikq(0)}, \quad (1)$$

occupies a pre-eminent position as it finds applications in the interpretation of experiments pertaining to different transport properties of solids, fluids, plasmas, etc [1]. Recently, Wierling and Swada [2] derived exact formulae for the dependence of CCF and its Laplace transform on time and wave-number for a particle in harmonic well of frequency Ω , which is an ideal case. They finally found that

$$Y(k, t) = \frac{\langle J_k^*(t) J_k(0) \rangle}{\langle |J_k(0)|^2 \rangle} = e^{-K(1 - \cos(\Omega t))} \{ \cos(\Omega t) - K \sin^2(\Omega t) \}, \quad (2) \text{ where } K = k^2 / m\beta\Omega^2. \text{ However, the actual systems are generally governed by anharmonic potentials, one of which is the cubic-quartic}$$

$$V(q) = m \left(\frac{\omega^2 q^2}{2} + \frac{aq^3}{3} + \frac{bq^4}{4} \right), \quad (3)$$

and has been extensively used in understanding some phenomena in solids and plasmas. Besides, $b = 0$ leads to the most studied Duffing oscillator. Srivastava and Vishwamittar [3] found that the approach developed in [4] was highly effective in determining quantum mechanical free energies of this system.

II. FORMULATION OF THE PROBLEM

With a view to use Eq. (2) for the cubic-quartic AHO, we have adapted the technique of [4] to the classical case, considered the reference harmonic potential $V_0(q) = \frac{1}{2} m \Omega^2 (q - a)^2$ and found the classical free energy

$$F \cong \frac{1}{\beta} \ln(\hbar\beta\Omega) + \langle V(q) - V_0(q) \rangle_0 \quad (4)$$

The expression so obtained

$$F = \left(\frac{1}{\beta}\right) kT \ln(\hbar\beta\Omega) + \frac{1}{2} m\omega^2 \alpha^2 + \frac{1}{3} m a \alpha^3 + \frac{1}{4} m b \alpha^4 + \left(\frac{1}{2} \beta \Omega^2\right) (\omega^2 + 2a\alpha + 3b\alpha^2 - \Omega^2) + \frac{3}{4} \frac{b}{m\beta^2 \Omega^4} \quad (5)$$

has been subjected to minimization w.r.t. α and Ω^2 yielding a pair of algebraic equations each in these parameters for a cubic ($b=0$), quartic ($a=0$) and cubic-quartic AHO. In all the cases α and Ω depend upon β . By determining these, we effectively reduce the actual problem of an AHO to that of a HO with eigenfrequency Ω and centered at α .

III. RESULTS AND DISCUSSION

The computations have been carried out for a good number of a , b and β values taking $\hbar/2\pi = m = \omega = 1$ and in double precision. It may be pointed out that for $m = 1$, the current correlation function numerically becomes the same as the velocity auto correlation function. The α and Ω values found as above have been then used to evaluate the relevant free energies from Eq. (5). These results have been, in turn, compared with the exact values for many cases employing the energy eigenvalues available in the literature [3 and references therein] and only those cases have been pursued for which the results for F differed by less than 3% from the actual values; this demanded $\beta < 0.5$. The Ω so determined have been employed to find the CCF $Y(k,t)$ and also its rates of variation with k and t , as function of wavenumber k for different values of inverse temperature and time using Eq. (2). The results for some typical cases have been projected in Figs. 1 - 4.

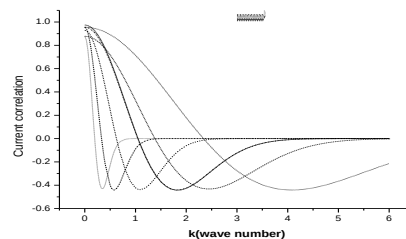


Fig. 1 Dependence of CCF on wavenumber k (from left to right) for HO [$t = 0.5$, $\beta = 0.01$], HO [$t = 0.3$, $\beta = 0.1$], cubic AHO [$a = 0.1$, $t = 0.5$, $\beta = 0.1$], HO [$t = 0.5$, $\beta = 0.5$], HO [$t = 0.3$, $\beta = 0.1$], cubic AHO [$a = 0.1$, $t = 0.3$, $\beta = 0.1$] and HO [$t = 0.3$, $\beta = 0.5$].

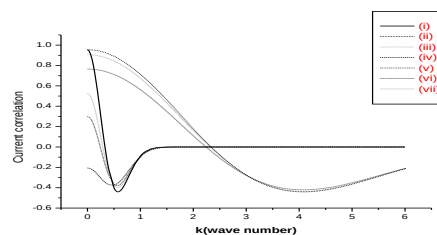


Fig. 2 CCF as function of wavenumber k at $t = 0.3$ (from left to right) for quartic AHOs {[$b = 4.0$, $\beta = 0.01$], [$b = 1.0$, $\beta = 0.01$], [$b = 0.4$, $\beta = 0.01$] }, HO [$\beta = 0.01$], quartic AHOs {[$b = 4.0$, $\beta = 0.5$], [$b = 0.4$, $\beta = 0.5$] }, and HO [$\beta = 0.5$].

It is seen from Eq. (2) that as function of time $Y(k,t)$ is periodic with the period $T = 2\pi/\Omega$ and is symmetric with respect to time π/Ω .

The only case where an oscillator with the kind of anharmonicities considered here has been studied is the quartic oscillator with $b = 1.0$ [5]. The agreement between the results of their analytical formalism and the numerical solutions was within 1 % for $\beta \sim 100$ and extremely poor for very low magnitudes of β so much so that for $\beta = 0.01$ there was no resemblance between the two. The latter exhibited a trend of variation in $Y(k,t)$ ($m=1$) with t somewhat similar to the amplitude of a damped oscillator. As regards the present effort, the CCF for this quartic AHO is periodic with $\Omega = 4.2223$ and can thus be taken in between the two extremes reported by them.

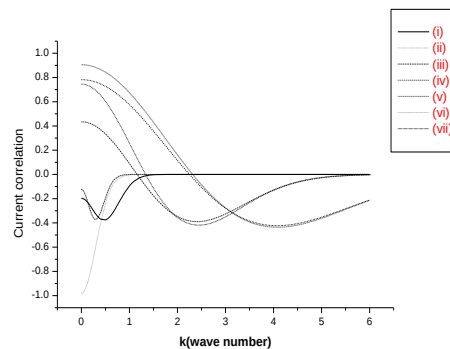


Fig. 3 Dependence of CCF on wavenumber k for various cubic – quartic oscillators (i) $a = 3.0$, $b = 4.0$, $t = 0.3$, $\beta = 0.01$, (ii) $a = 3.0$, $b = 4.0$, $t = 0.3$, $\beta = 0.5$, (iii) $a = 3.0$, $b = 4.0$, $t = 0.5$, $\beta = 0.01$, (iv) $a = 3.0$, $b = 4.0$, $t = 0.5$, $\beta = 0.5$, (v) $a = 0.03$, $b = 0.4$, $t = 0.5$, $\beta = 0.01$, (vi) $a = 0.3$, $b = 0.4$, $t = 0.3$, $\beta = 0.5$, (vii) $a = 0.03$, $b = 0.4$, $t = 0.5$, $\beta = 0.5$.

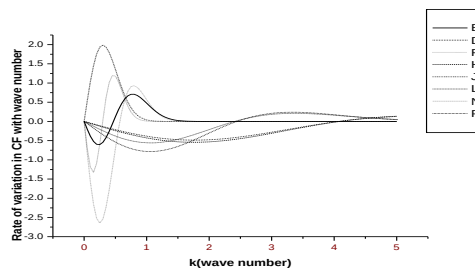


Fig. 4 The $\frac{\partial Y}{\partial k}$ as function of k for the cubic – quartic oscillators [$a = 3.0$, $b = 4.0$, $t = 0.3$, $\beta = 0.01$ (B); $a = 3.0$, $b = 4.0$, $t = 0.3$, $\beta = 0.5$ (D); $a = 0.03$, $b = 0.4$, $t = 0.3$, $\beta = 0.01$ (F); $a = 0.03$, $b = 0.4$, $t = 0.3$, $\beta = 0.5$ (H); $a = 3.0$, $b = 4.0$, $t = 0.5$, $\beta = 0.01$ (J); $a = 3.0$, $b = 4.0$, $t = 0.5$, $\beta = 0.5$ (L); $a = 0.03$, $b = 0.4$, $t = 0.5$, $\beta = 0.01$ (N); $a = 0.03$, $b = 0.4$, $t = 0.5$, $\beta = 0.5$ (P)].

IV. CONCLUSION

An exhaustive study has been carried out for the current correlation function of harmonic and anharmonic oscillators at different temperatures. These aspects need being pursued in more details employing other techniques and also other systems like harmonic and anharmonic chains, etc.

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