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Momentum autocorrelation function of an impurity in a classical oscillator chain with alternating masses III. Some limiting cases

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HIGHLIGHTS

- Momentum autocorrelation function of a mass impurity in a diatomic chain.
- 6 limiting cases where any of three masses approaches to zero or infinity.
- The cases $m_0 \to 0$ and $m_0 \to (2m_2)_+$ are closely related to each other.
- A quite different case $m_2 \to 0$ and its ergodicity.

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ABSTRACT

The momentum autocorrelation function of a mass impurity in a classic diatomic chain is studied using the recurrence relations method. General expressions for the contributions of branch cuts and resonant poles have been derived and illustrated in previous papers I and II, respectively. In the present paper a series of limiting cases that any one of the three masses m_0, m_1, m_2 approaches to zero or infinity are analyzed. It is found that the cases $m_0 \to 0$ and $\to (2m_2)_+$ are closely related to each other and that the general expressions for the amplitudes are valid also in the limits $\lambda \to 0$ and ∞. The ergodicity in the case $m_2 \to 0$ is studied and the ratio of two specific infinite products is obtained.

1. Introduction

It has a long history to study chains composed of classic harmonic oscillators as a model for dynamics of solids. Most of the early studies are conducted using the normal coordinate method [1,2]. Since developed in early 1980s, the recurrence relations (RR) method [3–5] has been used in various areas in physics [6–12] as well as in different models of oscillator chains [13–19].

In a previous paper [17, to be referred to as I] a chain composed of classic harmonic oscillators with alternating masses and a mass impurity is studied using the recurrence relations method. We have shown that the momentum autocorrelation function (ACF) of the impurity results from three branch cuts leading to acoustic and optical branches and from two pairs of resonant poles leading to cosine function(s). Two mass ratios $\eta = m_1/m_0$ and $\lambda = m_1/m_2$ are introduced as parameters of the model, where m_0 is the mass of the impurity and m_1, m_2 the masses of two kinds of oscillator in the chain. A $\eta - \lambda$ plane is introduced to characterize the model. Lines $\eta = \lambda$ and $\lambda = 1$ divide the $\eta - \lambda$ plane into four regions I_d, I_u, II_u and II_d. Whether a region is the physical region of the resonant mode μ or ν depends completely upon the values of η, λ. In

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different regions modes μ and ν may exist simultaneously or not, or even vanish both. The results are illustrated in detail [18, to be referred to as II], a frequency theorem and an envelope of the integrand of the cut contribution are also discussed.

In the present paper, a series of limiting cases are examined where any one of the three masses goes to zero or infinity while the other two are kept finite. Among them, $m_0 \to 0$ and $m_2 \to 0, \infty$ are studied in detail. The case $m_2 \to 0$ is quite different from all those we have studied before where the Hook constants are the *same*, so we need to study this case from the very beginning.

It is proved that the general expressions for the amplitudes M and N are also correct in the limits $\lambda \to 0$ and ∞, but not correct for M if $\eta \to 0$ and ∞.

In addition to the six limiting cases, we found that the case $\eta \to (\lambda/2)_+$ shares some features with that $\eta \to \infty$: In the two cases, the momentum ACFs have the same structure, they could be seen as the "image" of one another. The ergodicity in the case $m_2 \to 0$ is also discussed which leads to the evaluation of the ratio of two specific infinite products: $(\frac{1}{2}\frac{1}{2}\frac{1}{2}\cdots)/(\frac{1}{2}\frac{1}{2}\frac{1}{2}\cdots) = \frac{\sqrt{2}}{2}$.

In Section 2, general results of the model are briefly summarized. In Section 3 the six limiting cases are considered. The case $\eta \to (\lambda/2)_+$ is studied in Section 4. The ergodicity of the limiting case $m_2 \to 0$ is discussed in Section 5 and conclusions are drawn in Section 6.

2. General results of the model

In the formalism of recurrence relations (RR) method, a dynamical variable $A(t)$ can be expanded as [3–5]

$$A(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu, \tag{2.1}$$

where $\{f_\nu, \nu = 0, 1, 2, \ldots, d-1\}$ are a set of orthogonalized basis vectors which span a Hilbert space and coefficients $\{a_\nu(t)\}$ are a set of real functions bearing the time dependence of $A(t)$. The basis vectors $\{f_\nu\}$ satisfy recurrence relations:

$$f_{\nu+1} = Lf_\nu + \Delta_\nu f_{\nu-1}, \quad (\nu \geq 0, f_{-1} = 0, \Delta_0 \equiv 1),$$

with $L = i\{H, \}$ the Liouvillian of the system. The Hamiltonian H is Hermitian and $\Delta_\nu = \|f_\nu\|/\|f_{\nu-1}\|$ are the recurrants, $\|f_\nu\| = (f_\nu, f_\nu)$ is the norm of f_ν.

The Hilbert space S is realized by inner product (A, B) which is chosen as a classical ensemble average in our case:

$$(A, B) = \prod_i \int \mathrm{d}p_i\, \mathrm{d}q_i\, \mathrm{e}^{-\beta H} AB \Big/ \prod_i \mathrm{d}p_i\, \mathrm{d}q_i\, \mathrm{e}^{-\beta H}. \tag{2.2}$$

The realized space S is characterized by dimension d and $\{\Delta_\nu\}$ which may be finite or denumerably infinite depending on the model considered. In our case, the number of oscillators $N \to \infty$, so are the dimension d of space S and the recurrants $\{\Delta_\nu\}$.

Generally, the Laplace transform of $a_0(t)$ can be expressed in terms of the recurrants in the form of a continued fraction:

$$a_0(z) = 1/z + \Delta_1/z + \Delta_2/z + \cdots. \tag{2.3}$$

Therefore, if taking momentum of the impurity p_0 as f_0, we can calculate basis vectors f_ν, the norms, recurrants Δ_ν, $a_0(z)$ and $a_0(t)$ as well as momentum ACF $\langle p_0(t)p_0\rangle$.

We have used the recurrence relations method to study the momentum ACF of a mass impurity m_0 in a diatomic chain composed of classic harmonic oscillators with masses m_1, m_2, interacting only with nearest neighbors under periodic boundary conditions [17]. The impurity m_0 locates at site q_0 and the rest oscillators m_1, m_2 at q_{j_o} ($j_o = \pm 1, \pm 3, \ldots$) and q_{j_e} ($j_e = \pm 2, \pm 4, \ldots$), respectively. The oscillators interact with the nearest neighbors through Hook constant K. The model chain is characterized by the following Hamiltonian:

$$H = \frac{p_0^2}{2m_0} + \frac{1}{2m_1}\sum_{j_o} p_{j_o}^2 + \frac{1}{2m_2}\sum_{j_e} p_{j_e}^2 + \frac{K}{2}[(q_0 - q_1)^2 + (q_1 - q_2)^2 + \cdots + (q_{-2} - q_{-1})^2 + (q_{-1} - q_0)^2]. \tag{2.4}$$

The frequencies of the oscillators are determined by $\omega_i^2 = K/m_i (i = 0, 1, 2)$. If choose $K = m_1 = 1$, then $\omega_0^2 = \eta, \quad \omega_1^2 = 1, \omega_2^2 = \lambda$.

The basis vectors, norms and recurrants are calculated, some of them are listed in Table 1, where k_B is the Boltzmann constant, T the temperature.

The recurrants form a periodic sequence:

$$N \to \infty : \sigma = (2\eta, 1, 1, \lambda, \lambda, 1, 1, \lambda, \lambda, 1, 1, \lambda, \lambda, \ldots). \tag{2.5}$$

By (2.3) we have (I. 3.7–9)

$$a_0(z; \eta, \lambda) = \frac{(\eta - \lambda)P(z) + \eta S(z)}{D(z)} \tag{2.6}$$