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The Memory Function of an Impurity in Mass and Hooke Constant in a Diatomic Chain

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ABSTRACT

The memory function of an impurity with different mass and Hooke constant in a classical diatomic chain is studied by means of the recurrence relations method. The Laplace transform of the memory function has two pairs of resonant poles and three branch cuts. The poles contribute a cosine and the cuts contribute acoustic and optic branches, which are expressed as a convolution of a difference of two sines and an expansion of even-order Bessel functions. The expansion coefficients are integrals of Jacobian elliptic function sn(u) along the real axis in a complex u+iv plane for the acoustic branch, and integrals of nd(v) along a contour parallel to the imaginary axis of the plane for the optical branch, respectively. Different special cases are discussed in detail. It shows that a perfect monatomic or diatomic chain and such a chain with a mass impurity share the same memory function except for a constant factor, and that the pole contribution exists only if the impurity has both different mass and Hooke constant.

Keywords
Memory function, Impurity with different mass and Hooke constant, Diatomic chain, Resonant poles, Acoustic and optic branches, Jacobian elliptic functions.

Introduction
Harmonic oscillator chains are used as models in the study of solid-state physics [1-4]. The normal coordinates method was used in most of the early work. Since early 1980s the recurrence relations (RR) method has been developed [5-7] and applied to various areas in physics, for example, two-dimensional electron gas [8], a relativistic plasmonic Dirac electron gas [9] and spin dynamics of different models, etc. [10-14].

The RR method is also used to study oscillator chains, e.g., a monatomic chain without [15] or with a *mass* impurity [16], a Bethe lattice [17], a diatomic chains without [18] or with a *mass* impurity [19,20], a monatomic chain with a *full* impurity, i.e. an impurity with different *mass* and *Hooke constant* [21] as well as a diatomic chain with a *full* impurity [22], etc.

It is well known that a generalized Langevin equation involving a memory function was introduced by Mori [23] in a projection operator approach and was derived later by Lee using the RR method [7]. The memory function method has been applied to different physical models, such as the analysis of classical dense fluid and Heisenberg ferromagnets [7], spin-1/2 van der Waals model [24], two-dimensional dense electron gas at $T = 0$ [24,25], quantum one-dimensional *XY*-model [26], the long-time tail effect of the correlation function [27], as well as in solving the Liouville equation [28], etc. For a review of its applications c.f. [29]. The memory function of a full impurity in a monatomic chain is also studied by means of the RR method [21].

The purpose of this paper is to study the memory function of a full impurity in a classical diatomic chain. It turns out that the Laplace transform of the memory function has two pairs of resonant poles and three separate branch cuts. The poles contribute a cosine and the cuts contribute acoustic and optical branches. Both branches are expressed as a convolution of a difference of two sines and an expansion of even-order Bessel functions. The expansion coefficients are found the same as those obtained for the momentum autocorrelation function (ACF) of a *mass* impurity in a diatomic chain [20] except for a constant factor. Thus, we can directly employ the results of [20]. The expansion coefficients are integrals of Jacobian elliptic function $sn(u)$ along the real axis in a complex $u + iv$ plane for the acoustic branch, and integrals of elliptic function $nd(v)$ along a contour parallel to the imaginary axis in that plane for the optical branch, respectively.

The memory functions in different special cases are also examined. It turns out that the memory function of a chain with a *mass* impurity is the same as that of a *perfect* chain except for a constant factor, and that only if a chain has a *full* impurity has its memory function a contribution from the poles. These are true for both monatomic and diatomic chains.

The paper is organized as follows. In Section 2 an outline of the recurrence relations method is presented and the model is briefly studied in general. The pole and cut contributions to the memory function are respectively derived in Sections 3 and 4. Some special cases are examined in Section 5 and conclusions are drawn in Section 6.

Method and Model

In this section we briefly review the recurrence relations method and our model.

The Recurrence Relations Method

A dynamic variable $A(t)$ of a system may be expanded in a Hilbert space [5-7],

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

where $f_\nu \ (\nu = 0,1,\ldots,d-1)$ are orthogonal basis vectors which span a space S, the expansion coefficients $\{a_\nu(t)\}$ are real functions bearing the time dependence of $A(t)$. The vectors $\{f_\nu\}$ satisfy a set of recurrance relations

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

where L is the Liouvillian operator of the system, $\Delta_\nu = (f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1})$ are recurrants, and inner product $(A,B) = \prod_i \int dp_i dq_i e^{-\beta_T H} AB / \prod_i \int dp_i dq_i{}^{-\beta_T H}$ defines the space.

H is the Hamiltonian and β_T the inverse temperature. Similarly, $\{a_\nu(t)\}$ satisfy the flowing recurrence relations:

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t) \ \ (0 \leq \nu \leq d-1, \ a_{-1} \equiv 0)$$

with $a'_\nu(t) = da_\nu(t)/dt$. The time evolution of $A(t)$ is characterized by the dimensionality d of S and the recurrants $\sigma = (\Delta_1, \Delta_2, \ldots, \Delta_{d-1})$.

Now introduce a subspace S_1, which is spanned by basis vectors $\{f_1, f_2, \ldots, f_{d-1}\}$. A variable $B(t)$ in S_1 may be written as $B(t) = \sum_{\nu=1}^{d-1} b_\nu(t) f_\nu$, where $\{b_\nu(t)\}$ is a set of complete linear independent real functions satisfying the recurrence relations:

$$\Delta_{\nu+1} b_{\nu+1}(t) = -\dot{b}_\nu(t) + b_{\nu-1}(t) \ \ (1 \leq \nu \leq d-1, \ b_0 \equiv 0).$$

The Laplace transform of $b_1(t)$ may be expressed in terms of recurrants $\sigma_1 = (\Delta_2, \Delta_3, ,\ldots, \Delta_{d-1})$, a subset of σ:

$$b_1(z) = 1/(z + \Delta_2 /(z + \Delta_3 /(z + \ldots \Delta_{d-1} / z))). \qquad (2.1)$$

It is a continued fraction.

The time rate of $a_0(t)$ may be written as [7]

$$\dot{a}_0(t) = -\int_0^t d\tau \ \mathrm{M}(\tau) a_0(t-\tau).$$

It is a scalar generalized Langevin equation in which

$$\mathrm{M}(t) = \Delta_1 b_1(t) \qquad (2,2)$$

is the memory function.

The Model

A diatomic circle chain is composed of classic oscillators m_1, m_2 and an impurity m_0. Oscillators m_1 locate at sites $q_{\pm1,\pm3,\ldots}$, m_2 at $q_{\pm2,\pm4,\ldots}$ and m_0 at q_0. The oscillators m_1, m_2 are in interaction with their nearest neighbors via springs with Hooke constant *K,* and the impurity m_0 interacts with its two nearest neighbors m_1 through springs with Hooke constants K_0. The total oscillator number N is even. The periodic boundary conditions $q_{N/2} = q_{-N/2}$ and $\dot{q}_{N/2} = \dot{q}_{-N/2}$ are imposed.

The Hamiltonian of the model chain is given by

$$H = \frac{p_0^2}{2m_0} + \frac{1}{2m_1}\sum_{j_o} p_{j_o}^2 + \frac{1}{2m_2}\sum_{j_e} p_{j_e}^2 + \frac{K_0}{2}[\ q_0 - q_1)^2 + (q_{-1} - q_0)^2] +$$

$$+\frac{K}{2}[(q_1 - q_2)^2 + (q_2 - q_3)^2 + \cdots + (q_{-3} - q_{-2})^2 + (q_{-2} - q_{-1})^2]$$

The recurrants of the model $\sigma = (\Delta_1, \Delta_2, \Delta_3, \ldots, \Delta_{d-1})$ are derived as [22]

$$N \to \infty : \sigma = (2\eta\kappa, \kappa, 1, \lambda, \lambda, 1, 1, \lambda, \lambda, 1, 1, \lambda, \lambda, 1\ldots..), \qquad (2,3)$$

where $\eta = m_1/m_0$, $\lambda = m_1/m_2$ and $\kappa = K_0/K$ are parameters. σ is a sequence with periodicity four.

With (2.3), (2.1) reads

$b_1(z) = 1/(z + \kappa/(z + 1/(z + \lambda/(z + \lambda/(z + 1/(z \cdots))))))$

or $b_1(z) = 1/(z + \kappa / R)$, where

$R = z + 1/(z + \lambda/(z + \lambda/(z + 1/z + \ldots)))$, or

$R = z + 1/(z + \lambda/(z + \lambda/(z + 1/R)))$. It is a quadratic equation with solution $R = [z + S_0(z)]/2$,

$$S_0(z)=\sqrt{(z^2+2\lambda+2)(z^2+2)/(z^2+2\lambda)}, \quad (2.4)$$

thus

$$b_1(z)=\frac{z+S_0(z)}{z^2+2\kappa+zS_0(z)}. \quad (2.5)$$

After some algebra, we have

$$b_1(z)=\frac{1}{2}\frac{(\kappa-2)z^3+2(\kappa\lambda-\lambda-1)z+\kappa S(z)}{(\kappa-1)z^4+(\kappa^2+2\kappa\lambda-\lambda-1)z^2+2\kappa^2\lambda},$$

$$S(z)=\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}, \quad (2.6)$$

and

$$a^2=2(\lambda+1),\ b^2=2\lambda,\ c^2=2. \quad (2.7)$$

Write it as

$$b_1(z)=\frac{1}{2(\kappa-1)}\frac{(\kappa-2)z^3+p_1z+\kappa S(z)}{D(z)}, \quad (2.8)$$

where

$$p_1(z)=2(\kappa\lambda-\lambda-1), \quad (2.9)$$

$$D(z)=z^4+d_2z^2+d_0, \quad (2.10)$$

$$d_2=\frac{\kappa^2+2\kappa\lambda-\lambda-1}{\kappa-1},\ d_0=\frac{2\kappa^2\lambda}{\kappa-1} \quad (2.11)$$

are coefficients. $D(z)$ may be written as

$$D(z)=(z^2+m^2)(z^2+n^2), \quad (2.12)$$

$$m^2=\frac{d_2}{2}+\Delta,\ n^2=\frac{d_2}{2}-\Delta,\ \Delta=\sqrt{\frac{d_2^2}{4}-d_0}. \quad (2.13)$$

Thus we have

$$b_1(z;\kappa,\lambda)=\frac{1}{2(\kappa-1)}\frac{(\kappa-2)z^3+p_1z+\kappa\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}}{(z^2+m^2)(z^2+n^2)}. \quad (2.14)$$

It has two pairs of resonant poles $\pm im$, $\pm in$ and three branch cuts with endpoints at $\pm ia$, $\pm ib$ and $\pm ic$. Thus, we have

$$b_1(z;\kappa,\lambda)=b_1^{pol}(z;\kappa,\lambda)+b_1^{aco}(z;\kappa,\lambda)+b_1^{opt}(z;\kappa,\lambda), \quad (2.15a)$$

$$b_1(t;\kappa,\lambda)=b_1^{pol}(t;\kappa,\lambda)+b_1^{aco}(t;\kappa,\lambda)+b_1^{opt}(t;\kappa,\lambda). \quad (2.15b)$$

The initial condition is given by

$$b_1(0;\kappa,\lambda)=b_1^{pol}(0;\kappa,\lambda)+b_1^{aco}(0;\kappa,\lambda)+b_1^{opt}(0;\kappa,\lambda). \quad (2.16)$$

The Pole Contribution

Frequencies

By (2.14), we have

$$b_1^{pol}(t;\kappa,\lambda)=M\cos mt+N\cos nt,$$

with frequencies

$$m(\kappa,\lambda)=\sqrt{d_2/2+\Delta},\ n(\kappa,\lambda)=\sqrt{d_2/2-\Delta}. \quad (3.1)$$

The amplitudes *M* and *N* will be derived later. Besides, we obtain

(1) $m^2+n^2=d_2,\ m^2-n^2=2\Delta,\ m^2n^2=d_0$. (3.2)

(2) In the limit $\kappa\to1$,

$m^2(1_+,\lambda)=\lim_{\kappa\to1_+}m^2(\kappa,\lambda)\to\infty.$, $n^2(1,\lambda)=\lim_{\kappa\to1}n^2(\kappa,\lambda)=2$, or

$$m(1_+,\lambda)\to\infty,\ n(1,\lambda)=\sqrt{2}. \quad (3.3)$$

In this limit exists mode n only.

(3) Write (2.13) as

$$m^2(\kappa,\lambda)=\frac{1}{2(\kappa-1)}\left[A+\sqrt{A^2-B}\right],$$

$$n^2(\kappa,\lambda)=\frac{1}{2(\kappa-1)}\left[A-\sqrt{A^2-B}\right], \quad (3.4)$$

where

$$A=\kappa^2+2\kappa\lambda-\lambda-1,\ B=8\kappa^2(\kappa-1)\lambda,$$

$$\sqrt{A^2-B}=\sqrt{[\kappa^2-(2\kappa\lambda-\lambda-1)]^2+4\kappa^2(\lambda-1)}. \quad (3.5)$$

When $\lambda=1$:

$$m(\kappa,1)=\frac{\kappa}{\sqrt{\kappa-1}},\ n(\kappa,1)=\sqrt{2}. \quad (3.6)$$

When $\lambda=\kappa-1$:

$$m(\kappa,\kappa-1)=\sqrt{2\kappa},\ n(\kappa,\kappa-1)=\sqrt{\kappa}. \quad (3.7)$$

(4) Since m, n are frequencies, so m^2, n^2 must be real and non-negative:

$$\Delta^2\ge0,\ d_2^2\ge4d_0,\ \text{or}\ \Delta=0,\ d_2=2\sqrt{d_0} \quad (3.8)$$

determining a curve . At any point in the curve, the two frequencies are equal:

$$m_d^2=n_d^2=d_2/2. \quad (3.9a)$$

$$m_d(\kappa_d,\lambda_d)=n_d(\kappa_d,\lambda_d)=(d_2/2)^{1/2}=(d_0)^{1/4}. \quad (3.9b)$$

Frequencies $m(\kappa,\lambda)$ and $n(\kappa,\lambda)$ are plotted in Figures 1 and 2.

In Figure 1, when $\kappa\to1_+$, $m(\kappa,\lambda)\to\infty$ and $n(1,\lambda)=\sqrt{2}$, i.e. (3.3). All curves $n(\kappa,1)$ cross point $(1,\sqrt{2})$, c.f. (3.6). In Figure 2 we see something unexpected: Curve $m(4,\lambda)$ crosses $m(7,\lambda)$ at about $\lambda\approx4.5$, and it looks to cross $m(10,\ \lambda)$ somewhere outside the figure. This happens because $m(4,\lambda)$ has *larger* slope than $m(7,\lambda)$ and $m(10,\ \lambda)$ at, say, $\lambda=2$, 3, 4, etc.

Indeed, recall (3.4), we obtain

$$\frac{d}{d\lambda}m(\kappa,\lambda)=\frac{1}{4(\kappa-1)m}\left[2\kappa-1+\frac{(2\kappa-1)A-4\kappa^2(\kappa-1)}{\sqrt{A^2-B}}\right].$$

Then we numerically calculate and compare the slopes of $m(4,\ \lambda)$, $m(7,\ \lambda)$, $m(10,\ \lambda)$ with different values of λ and confirm that

$$\frac{d}{d\lambda}m(4,\lambda)>\frac{d}{d\lambda}m(7,\lambda)>\frac{d}{d\lambda}m(10.,\lambda)\ \text{at}\ \lambda=2,3,4,\text{etc.}$$

Thus with a given λ, $(d/d\lambda)m(\kappa,\lambda)$ decreases with increasing κ, so curve $m(\kappa,\lambda)$ becomes flatter with larger κ, i.e. curve $m(\kappa,\lambda)$ crosses those curves with larger κ.

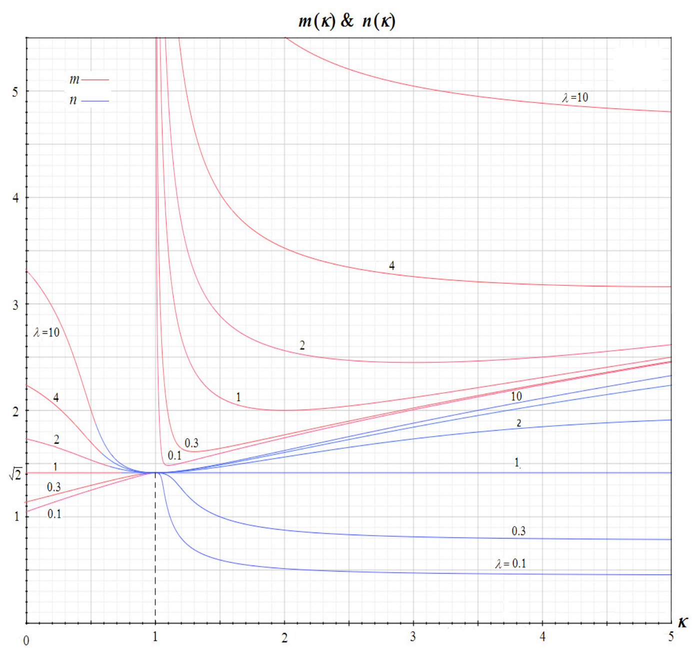

Figure 1: The κ- dependency of $m(\kappa)$ and $n(\kappa)$ with different λ.

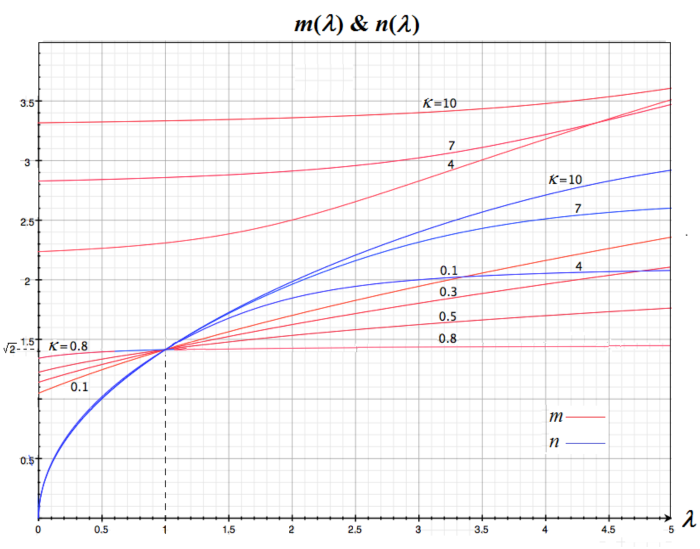

Figure 2: The λ - dependency of $m(\lambda)$ and $n(\lambda)$ with different κ.

Regions in the κ - λ plane

Now introduce a κ - λ plane. By (2.14), $b_1(z)$ has two pairs of resonant poles $\pm im$ and $\pm in$. We try to determine which mode, *m* or *n,* contributes to the memory function in a certain region.

Write (2.5) as

$$b_1(z) = \frac{z^3 + 2\lambda z + S(z)}{D_0(z) + zS(z)}, \tag{3.10}$$

$$D_0(z) = z^4 + 2(\kappa+\lambda)z^2 + 4\kappa\lambda \tag{3.11}$$

Thus we have

$$b_1(z;\kappa,\lambda) = \frac{z^3 + 2\lambda z + S(z)}{D_0(z) + zS(z)} = \frac{1}{2(\kappa-1)} \frac{(\kappa-2)z^3 + p_1 z + \kappa S(z)}{(z^2+m^2)(z^2+n^2)}.$$

At poles $\pm im$ and $\pm in$,

$$[D_0(z) + zS(z)]_{poles} = 0. \tag{3.12}$$

Introduce

$$D_0(m) \equiv D_0(\pm im) = m^4 - 2(\kappa+\lambda)m^2 + 4\kappa\lambda = (m^2 - 2\lambda)(m^2 - 2\kappa) \tag{3.13a}$$

$$D_0(n) \equiv D_0(\pm in) = n^4 - 2(\kappa+\lambda)n^2 + 4\kappa\lambda = (n^2 - 2\lambda)(n^2 - 2\kappa) \tag{3.13b}$$

In (3.12), the sign of $D_0(m)$ or $D_0(n)$ plays an important role in determining the mode *m* or *n*. Setting $D_0(m) = 0$ and $D_0(n) = 0$ yields m^2, $n^2 = 2\lambda, 2\kappa$. Setting $m^2 = 2\kappa$ yields $\kappa = 1$ and $\lambda = \kappa - 1$; setting $m^2 = 2\lambda$ gives $\lambda = 1$. Same are true for n^2. Thus, we have

$$\text{If } (m^2 \text{ or } n^2) = \begin{cases} 2\kappa \\ 2\lambda \end{cases}, \text{ then } \begin{cases} \kappa = 1, \quad \lambda = \kappa - 1 \\ \qquad\quad \lambda = 1 \end{cases}.$$

Lines $\lambda = 1$, $\kappa = 1$ and $\lambda = \kappa - 1$ divide the κ - λ plane into six regions III_d, III_u, II_d, II_u, I_d, and I_u shown in Figure 3.

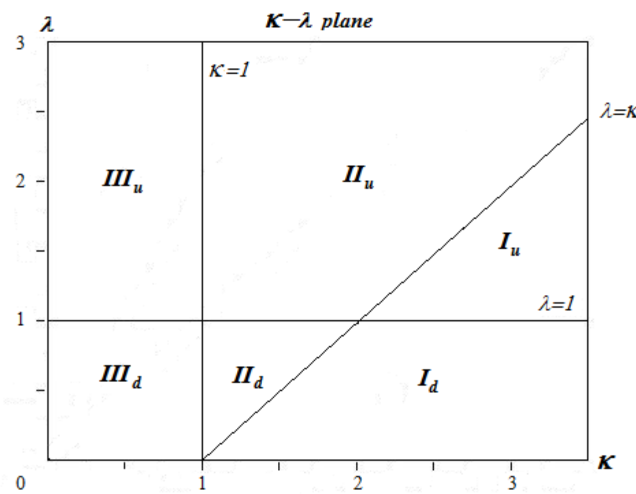

Figure 3: The regions in the κ - λ plane.

Numerical calculation of $D_m(\kappa,\lambda)$ and $D_n(\kappa,\lambda)$ gives their signs in the vicinities of lines $\lambda = 1$ and $\lambda = \kappa - 1$ listed in Table 1.

Table 1: Signs of $D_m(\kappa,\lambda)$, $D_n(\kappa,\lambda)$ in the vicinities of lines $\lambda = 1$ and $\lambda = \kappa - 1$.

Region	III_d	III_u	I_d	I_u	I_d	I_u
$D_m(\kappa,\lambda)$	+	-	+	+	-	-
$D_n(\kappa,\lambda)$	+	-	-	+	-	-

Amplitudes

In Appendix A, amplitudes *M* and *N* are derived by taking into account the signs of $D_m(\kappa,\lambda)$, $D_n(\kappa,\lambda)$ in (3.12) shown in Table 1 and calculating the residues of function

$$h(z)=\frac{1}{2(\kappa-1)}\frac{(\kappa-2)z^3+p_1z+\kappa\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}}{(z^2+m^2)(z^2+n^2)}e^{zt} \quad (3.14)$$

at poles $\pm im$ and $\pm in$ in different regions. The results are as follows:

$$M=\frac{(\kappa-2)m^2-p_1}{2(\kappa-1)\Delta}=\frac{\kappa\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}}{2(\kappa-1)\Delta m}, \quad (3.15a)$$

$$N=\frac{(2-\kappa)n^2+p_1}{2(\kappa-1)\Delta}=\frac{\kappa\sqrt{(n^2-a^2)(n^2-b^2)(n^2-c^2)}}{2(\kappa-1)\Delta n}. \quad (3,15b)$$

By (A.5a, b)~(A.10a, b), we have the mode and amplitude in different regions shown in Table 2.

Table 2: Mode and amplitude in different regions.

Region	III_d	III_u	I_d	I_u	I_d	I_u
Mode & Amplitude	*n, N*	*m. M*	*none*	*n, N*	*m, M*	*m, M*

Comparing Table 1 and Table 2 we reach the criteria:

In the physical region of mode *m* or *n*, respectively holds the inequality

$$D_m(\kappa,\lambda)<0\,,\ D_n(\kappa,\lambda)>0\,. \quad (3.16)$$

Therefore, the pole contribution in different regions are as follows:

$$b_1^{pol}(t;\kappa,\lambda<1)=\begin{cases}M\cos mt\\ N\cos nt\\ 0\end{cases} \text{in region} \begin{cases}I_d\\ III_d\\ I_d\end{cases}, \quad (3.17a)$$

$$b_1^{pol}(t;\kappa,\lambda>1)=\begin{cases}M\cos mt\\ N\cos nt\end{cases} \text{in region} \begin{cases}III_u, I_u\\ I_u\end{cases}. \quad (3.17b)$$

The amplitudes are subject to $|M(\kappa,\lambda)|\le 1$ and $|N(\kappa,\lambda)|\le 1$.

The Cut Contribution

Now consider the cut contribution to the memory function.
Since $(\kappa-2)z^3+p_1z$ in (2.14) contributes nothing to $b_1^{cut}(t)$, thus

$$b_1^{cut}(t;;\kappa,\lambda)=\frac{\kappa}{2(\kappa-1)}\,\mathrm{L}^{-1}\left[\frac{\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}}{(z^2+m^2)(z^2+n^2)}\right], \quad (4.1)$$

here L denotes the Laplace transformation.
Write the integrand as $f(z)g(z)$, take $f(z)=[(z^2+m^2)(z^2+n^2)]^{-1}$ and $g(z)=\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}$, then

$$F(t)=\mathrm{L}^{-1}[f(z)]=\frac{m\sin nt-n\sin mt}{mn(m^2-n^2)}, \quad (4.2)$$

$$G(t)=\mathrm{L}^{-1}[g(z)]=\frac{1}{2\pi i}\oint_C dz\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}e^{zt},$$

and

$$b_1^{cut}(t)=\frac{\kappa}{2(\kappa-1)}\int_0^t d\tau F(t-\tau)G(\tau)=\frac{\kappa}{2(\kappa-1)}\int_0^t d\tau F(\tau)G(t-\tau). \quad (4.3)$$

Here $G(t)$ depends only on λ, i.e. independent of the impurity. Moreover, (4.3) is the same as Eq. (18b) in Ref. [20] except for a constant factor $\alpha=\eta/(2\eta-\lambda)$, so we can write down $G(t)$ directly. In the following we refer Ref. [20] as I and denote, say, Eq. (18b) in Ref. [20] as Eq. (I.18b), etc.

Acoustic branch

If $\lambda<1$ $(0\le y\le b<c<a)$. By (I.41a),

$$G^{aco}(t;\lambda<1)=\frac{2ab^2c}{\pi}[U_0^{aco}(\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda<1)J_{2n}(bt)], \quad (4.4)$$

where $\{c_j(n)\}$ are expansion coefficients, $U_0^{aco}(\lambda<1)$ and $\tilde{U}_j^{aco}(\lambda<1)$ are auxiliary integrals, their expressions and relevant quantities are respectively given by Eqs. (I.36) and (I.40) etc. Thus the acoustic branch is

$$b_1^{aco}(t;\kappa,\lambda<1)=\frac{ab^2c\kappa}{\pi(\kappa-1)mn(m^2-n^2)}\int_0^t d\tau[m\sin n(t-\kappa)-n\sin m(t-\kappa)]\times$$
$$[U_0^{aco}(\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda<1)J_{2n}(b\tau)]. \quad (4.5)$$

If $\lambda>1$ $(0\le y\le c<b<a)$. By (I.56a),

$$G^{aco}(t;\lambda>1)=\frac{2abc^2}{\pi}[U_0^{aco}(\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda>1)J_{2n}(ct)], \quad (4.6)$$

where $U_0^{aco}(\lambda>1)$ and $\tilde{U}_j^{aco}(\lambda>1)$ are given by (I.51) and (I.55), respectively.

The acoustic branch is thus

$$b_1^{aco}(t;\kappa,\lambda>1)=\frac{abc^2\kappa}{\pi(\kappa-1)mn(m^2-n^2)}\int_0^t d\tau[m\sin n(t-\kappa)-n\sin m(t-\kappa)]\times$$
$$[U_0^{aco}(\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda>1)J_{2n}(c\tau)]. \quad (4.7)$$

The acoustic branch is expressed as a convolution of a difference of two sines and an even-order Bessel function expansion. The expansion coefficients are integrals of elliptic function $sn(u)$ along the real axis in a complex $u+iv$ plane. Besides, $U_0^{aco}(\lambda)$ can be expressed in terms of Legendre elliptic integrals of the first, second and third kind [20].

Optical Branch

If $\lambda<1$ $(0<b<c\le y\le a)$. By (I.77a),

$$G^{opt}(t;\lambda<1)=\frac{2a^2bc}{\pi}[V_0^{opt}(\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda<1)J_{2n}(at)]. \quad (4.8)$$

Integrals $V_0^{opt}(\lambda<1)$, $\tilde{V}_j^{opt}(\lambda<1)$ and relevant quantities are respectively shown in Eqs. (I.73) and (I.76), etc. The optical branch reads

$$b_1^{opt}(t;\kappa,\lambda<1)=\frac{a^2bc\kappa}{\pi(\kappa-1)mn(m^2-n^2)}\int_0^t d\tau[m\sin n(t-\kappa)-n\sin m(t-\kappa)]\times$$
$$[V_0^{opt}(\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda<1)J_{2n}(a\tau)]. \quad (4.9)$$

If $\lambda>1$ $(0<c<b\le y\le a)$. By (I.88a),

$$G^{opt}(t;\lambda>1)=\frac{2a^2bc}{\pi}[V_0^{opt}(\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda>1)J_{2n}(at)], \quad (4.10)$$

and auxillary integrals $V_0^{opt}(\lambda>1)$ and $\tilde{V}_j^{opt}(\lambda>1)$ are given by (I.85) and (I.86), respectively.

The optical branch takes the form

$$b_1^{opt}(t;\kappa,\lambda>1)=\frac{a^2bc\kappa}{\pi(\kappa-1)mn(m^2-n^2)}\int_0^t d\tau[m\sin n(t-\kappa)-n\sin m(t-\kappa)]\times$$

$$[V_0^{opt}(\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda>1)J_{2n}(a\tau)]. \quad (4.11)$$

The optical branch is given by a convolution of a difference of two sines and an even-order Bessel function expansion. The expansion coefficients are integrals of elliptic functions *nd*(v) along a contour parallel to the imaginary axis in the complex $u+iv$ plane.

In fact, the expansion coefficients for the optical branch are originally obtained as integrals of complex elliptic functions *sn*($u+iv$). By means of the addition theorem [30], the complex elliptic function is replaced by a real function *nd*(v).

Finally, we obtain the memory functions

$$\mathrm{M}(t;\kappa,\lambda<1)=2\eta\kappa[b_1^{pol}(t;\kappa,\lambda<1)+b_1^{aco}(t;\kappa,\lambda<1)+b_1^{opt}(t;\kappa,\lambda<1)]. \quad (4.12a)$$

$$\mathrm{M}(t;\kappa,\lambda>1)=2\eta\kappa[b_1^{pol}(t;\kappa,\lambda>1)+b_1^{aco}(t;\kappa,\lambda>1)+b_1^{opt}(t;\kappa,\lambda>1)]. \quad (4.12b)$$

Since the cut contribution is given by a convolution, the initial condition (2.16) is not appropriate. However, after the time integral is worked out, (2.16) applies.

Special cases

Now consider some special cases, which are identified by parameters (η,κ,λ). For example, a quantity Q pertaining to a chain characterized by (η,κ,λ) is denoted by $Q(\eta,\kappa,\lambda)$, etc.

$\eta=\kappa=\lambda=1$

This is a *perfect* monatomic chain composed of infinite oscillators of mass m interacting with their nearest neighbors through K. Its recurrants are $\sigma(1,1,1)=(2,1,1,1,...)$, and subset $\sigma_1(1,1,1)=(1,1,1,...)$.

$$b_1(z;1,1,1)=(1/2)\left[-z+\sqrt{z^2+4}\right]. \quad (5.1)$$

It has a branch cut between [-2, 2] but no poles. Thus

$$b_1(t;1,1,1)=\frac{1}{\pi}\int_0^2 dy\sqrt{4-y^2}\cos(yt).$$

Set $y=2\sin\theta$, then $b_1(t;1,1,1)=(4/\pi)\int_0^{\pi/2}d\theta\cos^2\theta\cos(2t\cos\theta)$

Making use of

$$\cos(at\sin\theta)=J_0(at)+2\sum_{n=1}^{\infty}J_{2n}(at)\cos(2n\theta), \quad (5.2)$$

we obtain

$$b_1(t;1,1,1)=\frac{4}{\pi}\left[U_0(1,1,1)J_0(2t)+2\sum_{n=1}^{\infty}U_n(1,1,1)J_{2n}(2t)\right], \quad (5.3a)$$

where

$$U_n(1,1,1)=\int_0^{\pi/2}d\theta\cos^2\theta\cos(2n\theta)\ \ (n=0,1,2,...). \quad (5.3b)$$

Thus

$$U_0(1,1,1)=\int_0^{\pi/2}d\theta\cos^2\theta=\frac{\pi}{4}, \quad (5.4a)$$

$$U_n(1,1,1)=\frac{\pi}{4}+\sum_{j=1}^{n}c_j(n)\int_0^{\pi/2}d\theta\cos^2\theta\sin^{2j}\theta\ \ (n=1,2,...), \quad (5.4b)$$

where the following formulae are used:

$$\cos(2n\theta)=1+\sum_{j=1}^{n}c_j(n)\sin^{2j}\theta\ \ (n=1,2,...), \quad (5.5a)$$

$$c_1=-\frac{4n^2}{2!},\ c_2=\frac{4n^2(4n^2-2^2)}{4!},\ c_3=-\frac{4n^2(4n^2-2^2)(4n^2-4^2)}{6!},... \quad (5.5b)$$

Hence we obtain

$$b_1(t;1,1,1)=1+\frac{8}{\pi}\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\int_0^{\pi/2}d\theta\cos^2\theta\sin^{2j}\theta\ J_{2n}(\mu t), \quad (5.6)$$

where

$$J_0(2t)+2\sum_{n=1}^{\infty}J_{2n}(2t)=1 \quad (5.7)$$

is used. Thus the memory function is

$$\mathrm{M}(t;1,1,1)=\Delta_1(1,1,1)b_1(t;1,1,1)$$
$$=2\left[1+\frac{8}{\pi}\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\int_0^{\pi/2}d\theta\cos^2\theta\sin^{2j}\theta J_{2n}(2t)\right]. \quad (5.8)$$

$\kappa=\lambda=1$

This is a monatomic chain with a *mass* impurity m_0. Its recurrants are $\sigma(\eta,1,1)$ = $(2\eta,1,1,1,1)$, $\Delta_1(\eta,1,1)=2\eta$, $\sigma_1(\eta,1,1)=(1,1,1,1,...)$, it is the same as $\sigma_1(1,1,1)$. $b(z;\eta,1,1)$ has no poles but a cut, and $b_1(t;\eta,1,1)=b_1(t;1,1,1)$ given by (5.6). The memory function is then

$$\mathrm{M}(t;\eta,1,1)=\Delta_1(\eta,1,1)b_1(t;\eta,1,1)$$
$$=2\eta\left[1+\frac{8}{\pi}\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\int_0^{\pi/2}d\theta\cos^2\theta\sin^{2j}\theta J_{2n}(2t)\right]. \quad (5.9)$$

$\lambda=1$

This is a monatomic chain composed of oscillators m and a *full* impurity $m_0=m/\eta$. The oscillators m interact with their nearest neighbors through K while the impurity m_0 interacts with its two nearest neighbors through $K_0=\kappa K$. This case is studied [21] and its memory function is [31]

$$\mathrm{M}(t;\eta,\kappa,1)=2\eta\kappa\left\{M(\kappa,1)\cos(\mu t)+\frac{1}{\sqrt{\kappa-1}}\int_0^t d\tau\sin\mu(t-\tau)[J_0(2\tau)+J_2(2\tau)]\right\}, \quad (5.10)$$

where $\mu=\kappa/\sqrt{\kappa-1}$ is the frequency and $M(\kappa,1)=(\kappa-2)/(\kappa-1)$ is the amplitude of the resonant vibration.

$\eta=\kappa=1$

This is a *perfect* diatomic chain composed of two kinds of oscillators m_1,m_2 interacting with their nearest neighbors through Hooke constant K. Choose one oscillator m_2 as m_0: $m_0=m_2$, then $\eta=m_1/m_0=m_1/m_2=\lambda$. Its recurrants are given by $\sigma(1,1,\lambda)=(2\lambda,1,1,\lambda,\lambda,1,1,\lambda,\lambda,...)$

[18], $\Delta_1(1,1,\lambda)=2\lambda$, and $\sigma_1(1,1,\lambda)=(1,1,\lambda,\lambda,1,1,\lambda,\lambda,...)$. Thus

$$b_1(z;1,1,\lambda)=-\frac{1}{2\lambda}\frac{z^3+2z-\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}}{z^2+2}. \quad (5.11)$$

It has a pair of poles $\pm i\sqrt{2}$ and three branch cuts. However, the residues of $b_1(z;1,1,\lambda)$ at poles $\pm i\sqrt{2}$ are found zero, $b_1^{pol}(t;1,1,\lambda)=0$. Hence $b_1(t;1,1,\lambda)$ results from three cuts only: $b_1(z;1,1,\lambda)=b_1^{cut}(z;1,1,\lambda)$. Since $c^2=2$, so

$$b_1(t;1,1,\lambda)=\frac{1}{2\lambda}\frac{1}{2\pi i}\oint dz\,\bar{b}_1(z;1,1,\lambda)e^{zt}. \quad (5.12)$$

where

$$\bar{b}_1(z;1,1,\lambda)=\sqrt{\frac{(z^2+a^2)(z^2+b^2)}{z^2+c^2}}. \quad (5.13)$$

Set $\bar{b}_1(z)=f(z)g(z)$, $f(z)=1/\sqrt{z^2+c^2}$, $g(z)=\sqrt{(z^2+a^2)(z^2+b^2)}$, then

$F(t)=L^{-1}[f(z)]=J_0(ct)$, $G(t)=L^{-1}[g(z)]$ and

$$b_1(t;1,1,\lambda)=\frac{1}{2\lambda}\int_0^t d\tau J_0(ct-c\tau)G(\tau). \quad (5.14)$$

Next we calculate $G(t)$ with different λ.

Acoustic branch

For $\lambda<1$ $(0\le y\le b<c<a)$ we have

$$G^{aco}(t;1,1,\lambda<1)=\frac{2}{\pi}\int_0^b dy\sqrt{(a^2-y^2)(b^2-y^2)}\cos(yt).$$

Setting $y=b\sin\theta$ and making use of (5.2) yield

$$G^{aco}(t;1,1,\lambda<1)=\frac{2ab^2}{\pi}[U_0^{aco}(1,1,\lambda<1)J_0(bt)+2\sum_{n=1}^{\infty}U_n^{aco}(1,1,\lambda<1)J_{2n}(bt)], \quad (5.15)$$

the auxiliary integrals are

$$U_n^{aco}(1,1,\lambda<1)=\int_0^{\pi/2}d\theta\sqrt{1-k^2\sin^2\theta}\cos^2\theta\cos(2n\theta)$$

$$(n=0,1,2,\cdots,\ k^2=(b/a)^2=\lambda(\lambda+1)<1). \quad (5.16)$$

We have

$$U_0^{aco}(1,1,\lambda<1)=\int_0^{K(k)}du\ cn^2(u,k)dn^2(u,k), \quad (5.17)$$

where $cn(u,k)$, $dn(u,k)$, are Jacobian elliptic functions and $K(k)$ the complete Legendre elliptic integral of the first kind. Making use of (5.5) we get

$$U_n^{aco}(1,1,\lambda<1)=U_0^{aco}(1,1,\lambda<1)+\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(1,1,\lambda>1)\ (n=1,2,...) \quad (5.18a)$$

$$\tilde{U}_j^{aco}(1,1,\lambda<1)=\int_0^{K(k)}du\ cn^2(u,k)dn^2(u,k)sn^{2j}(u,k). \quad (5.18b)$$

Then (5.15) becomes

$$G^{aco}(t;1,1,\lambda<1)=\frac{2ab^2}{\pi}\left[U_0^{aco}(1,1,\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(1,1,\lambda<1)J_{2n}(bt)\right], \quad (5.19)$$

where (5.7) is used. Hence, the acoustic contribution is given by

$$b_1^{aco}(t;1,1,\lambda<1)=\frac{ab^2}{\pi\lambda}\int_0^t d\tau J_0(ct-c\tau)\left[U_0^{aco}(1,1,\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(1,1,\lambda<1)J_{2n}(b\tau)\right]. \quad (5.20)$$

For $\lambda>1$ $(0\le y\le c<b<a)$, we have

$G^{aco}(t;1,1,\lambda>1)=\frac{2}{\pi}\int_0^c dy\sqrt{(a^2-y^2)(b^2-y^2)}\cos(yt)$. Set $y=c\sin\theta$, then

$$G^{aco}(t;,1,1,\lambda>1)=\frac{2abc}{\pi}[U_0^{aco}(1,1,\lambda>1)J_0(ct)+2\sum_{n=1}^{\infty}U_n^{aco}(1,1,\lambda>1)J_{2n}(ct)]. \quad (5.21)$$

The auxiliary integrals are

$$U_n^{aou}(1,1,\lambda>1)=\int_0^{\pi/2}d\theta\sqrt{(1-l_1^2\sin\theta)(1-l_2^2\sin\theta)}\cos\theta\cos(2n\theta)$$

$$(n=0,1,2,...,), \quad (5.22a)$$

$$l_1^2=(c/b)^2=1/\lambda<1,\ l_2^2=(c/a)^2=1/(\lambda+1)<1,\ 0<l_2^2<l_1^2<1. \quad (5.22b)$$

In Appendix B, we get

$$U_0^{aco}(1,1,\lambda>1)=(1-l_2^2)^2\int_0^{K(l)}du\frac{cn(u,l)dn^2(u,l)}{[1-l_2^2cn^2(u,l)]^{5/2}}, \quad (5.23a)$$

$$U_n^{aco}(1,1,\lambda>1)=U_0^{aco}(1,1,\lambda>1)+\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{opt}(1,1,\lambda>1), \quad (5.23b)$$

$$\tilde{U}_j^{aco}(1,1,\lambda>1)=(1-l_2^2)^2\int_0^{K(l)}du\frac{cn(u,l)dn^2(u,l)sn^{2j}(u,l)}{[1-l_2^2cn^2(u,l)]^{j+5/2}}, \quad (5.23c)$$

where $l^2=(l_1^2-l_2^2)/(1-l_2^2)=1/\lambda<1$ and $K(l)$ is the complete Legendre elliptic integral of the first kind.

Thus (5.21) reads

$$G^{aco}(t;1,1,\lambda>1)=\frac{2abc}{\pi}\left[U_0^{aco}(1,1,\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(1,1,\lambda>1)J_{2n}(ct)\right], \quad (5.24)$$

in which (5.7) is used.

The acoustic contribution is then given by

$$b_1^{aco}(t;1,1,\lambda>1)=\frac{abc}{\pi\lambda}\int_0^t d\tau J_0(ct-c\tau)\left[U_0^{aco}(1,1,\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(1,1,\lambda>1)J_{2n}(c\tau)\right] \quad (5.25)$$

In (5.20) or (5.25), $b_1^{aao}(t;1,1,\lambda)$ is expressed as a convolution of a zero-order Bessel function and an even-order Bessel function expansion. The expansion coefficients are integrals of Jacobian elliptic functions.

Optical branch

If $\lambda<1$ $(0<b<c\le y\le a)$, then

$G^{opt}(t;1,1,\lambda<1)=\frac{2}{\pi}\int_c^a dy\sqrt{(a^2-y^2)(b^2-y^2)}\cos(yt)$. By $y=a\sin\theta$ and (5.2),

$$G^{opt}(t;1,1,\lambda<1)=\frac{2a^2b}{\pi}[V_0^{opt}(1,1,\lambda<1)J_0(at)+2\sum_{n=1}^{\infty}V_n^{opt}(1,1,\lambda<1)J_{2n}(at)],$$

where

$$V_n^{opt}(1,1,\lambda<1)=\int_{\theta_c}^{\pi/2}d\theta\sqrt{1-r^2\sin^2\theta}\cos^2\theta\cos(2n\theta)$$

$$(n=0,1,2,...,r^2=(a/b)^2=(\lambda+1)/\lambda>1). \quad (5.26)$$

are auxiliary integrals. In Appendix C, we derive that

$$V_0^{opt}(1,1,\lambda<1) = -ip(p')^4 \int_{v_c}^{K(p')} dv\ cd^2(v,p') sd^2(v,p'). \quad (5.27a)$$

$$V_n^{opt}(1,1,\lambda<1) = V_0^{opt}(1,1,\lambda<1) + \sum_{j=1}^{n} c_j(n) \tilde{V}_j^{opt}(1,1,\lambda<1). \quad (5.27b)$$

$$\tilde{V}_j^{opt}(1,1,\lambda<1) = -ip^{2j+1}(p')^4 \int_{v_c}^{K(p')} dv\ cd^2(v,p') sd^2(v,p') nd^{2j}(v,p'). \quad (5.27c)$$

Thus

$$G^{opt}(t;1,1,\lambda<1) = \frac{2a^2 b}{\pi}\left[V_0^{opt}(1,1,\lambda<1) + 2\sum_{n=1}^{\infty}\sum_{j=1}^{n} c_j(n)\tilde{V}_j^{opt}(1,1,\lambda<1) J_{2n}(at)\right] \quad (5.28)$$

and the optical branch is

$$b_1^{opt}(t;1,1,\lambda<1) = \frac{a^2 b}{\pi\lambda}\int_0^t d\tau J_0(ct-c\tau)\left[V_0^{opt}(1,1,\lambda<1) + 2\sum_{n=1}^{\infty}\sum_{j=1}^{n} c_j(n)\tilde{V}_j^{opt}(1,1,\lambda<1) J_{2n}(a\tau)\right] \quad (5.29)$$

If $\lambda > 1$ $(0 < c < b \le y \le a)$, then

$$G^{opt}(t;1,1,\lambda>1) = \frac{2}{\pi}\int_b^a dy \sqrt{(a^2-y^2)(b^2-y^2)} \cos^2\theta \cos(yt).$$

Similarly, set $y = a\sin\theta$ $(\sin\theta_b = b/a)$, then

$$G^{opt}(t;1,1,\lambda>1) = \frac{2a^2 b}{\pi}[V_0^{opt}(1,1,\lambda>1) J_0(at) + 2\sum_{n=1}^{\infty} V_n^{opt}(1,1,\lambda>1) J_{2n}(at)], \quad (5.30)$$

with

$$V_n^{opt}(1,1,\lambda>1) = \int_{\theta_b}^{\pi/2} d\theta \sqrt{1-r^2\sin^2\theta}\cos^2\theta\cos(2n\theta)$$

$$(n = 0,1,2,..., r^2 = (a/b)^2 = (\lambda+1)/\lambda > 1). \quad (5.31)$$

The only difference between (5.31) and (5.26) lies at the lower limit of integration. Thus (5.30) reads

$$G^{opt}(t;1,1,\lambda>1) = \frac{2a^2 b}{\pi}\left[V_0^{opt}(1,1,\lambda>1) + 2\sum_{n=1}^{\infty}\sum_{j=1}^{n} c_j(n)\tilde{V}_j^{opt}(1,1,\lambda>1) J_{2n}(at)\right]. \quad (5.32)$$

In Appencix C, the auxiliary integtals are obtained as

$$V_0^{opt}(1,1,\lambda>1) = -ip(p')^4 \int_0^{K(p')} dv\ cd^2(v.p') sd^2(v.p'), \quad (5.33a)$$

$$\tilde{V}_j^{opt}(1,1,\lambda>1) = -ip^{2j+1}(p')^4 \int_0^{K(p')} dv\ cd^2(v,p') sd^2(v,p') nd^{2j}(v,p'). \quad (5.33b)$$

So we have the optical branch

$$b_1^{opt}(t;1,1,\lambda>1) = \frac{a^2 b}{\pi\lambda}\int_0^t d\tau J_0(ct-c\tau)\left[V_0^{opt}(1,1,\lambda>1) + 2\sum_{n=1}^{\infty}\sum_{j=1}^{n} c_j(n)\tilde{V}_j^{opt}(1,1,\lambda>1) J_{2n}(a\tau)\right]. \quad (5.34)$$

In (5.29) or (5.34), the optical branch is given by a convolution of a zero-order Bessel function and an even-order Bessel function expansion. The expansion coefficients are integrals of Jacobian elliptic functions along a contour $u = K(p)$ parallel to the imaginary axis in the u+iv plane.

In addition, the modulus of the elliptic functions in the two branches are related to each other.

In fact, if $\lambda < 1$, $k^2 = p^2 = \lambda/(\lambda+1)$, thus k and p' are complementary to each there; if $\lambda > 1 \cdot l^2 = 1/\lambda \cdot p' = \lambda/\sqrt{l^2+1}$, l and p' are related to each other also.
Therefore, the memory function of a *perfect* diatomic chain is as follows:

$$\mathrm{M}(t;1,1,\lambda<1) = 2\lambda\left[b_1^{aco}(t;1,1,\lambda<1) + b_1^{opt}(t;1,1,\lambda<1)\right], \quad (5.35a)$$

$$\mathrm{M}(t;1,1,\lambda>1) = 2\lambda\left[b_1^{aco}(t;1,1,\lambda>1) + b_1^{opt}(t;1,1,\lambda>1)\right]. \quad (5.35b)$$

$\kappa = 1$

This is a diatomic chain composed of oscillators of masses m_1, m_2 and a *mass* impurity m_0. All oscillators interact with their nearest neighbors through Hooke constant K. The recurrants are given by $\sigma(\eta,1,\lambda) = (2\eta,1,1,\lambda,\lambda,1,1,\lambda,\lambda,...)$, $\Delta_1(\eta,1,\lambda) = 2\eta$, and $\sigma_1(\eta,1,\lambda) = (1,1,\lambda,\lambda,1,1,\lambda,\lambda,...)$, the same as $\sigma_1(1,1,\lambda)$, hence $b_1(t;\eta,1,\lambda) = b_1(t;1,1,\lambda)$.

Therefore, the memory functions of this chain are given by

$$\mathrm{M}(t;\eta,1,\lambda<1) = 2\eta\left[b_1^{aco}(t;\eta.1.\lambda<1) + b_1^{opt}(t;\eta,1,\lambda<1)\right], \quad (5.36a)$$

$$\mathrm{M}(t;\eta,1,\lambda>1) = 2\eta\left[b_1^{aco}(t;\eta.1.\lambda>1) + b_1^{opt}(t;\eta,1,\lambda>1)\right] \quad (5.36b)$$

where $b_1^{aco}(t;\eta,1,\lambda<1)$, $b_1^{opt}(t;\eta,1,\lambda<1)$, and $b_1^{aco}(t;\eta,1,\lambda>1)$, $b_1^{opt}(t;\eta,1,\lambda>1)$ are given by (5.20), (5.29) and (5.25), (5.34), respectively.

Discussion

In the proceeding sections, we have examined memory functions of different chains. We find that a *perfect* monatomic chain $(1,1,\lambda)$ and a monatomic chain with a *mass* impurity $(\eta,1,\lambda)$ have the same $\sigma_1(111) = \sigma_1(\eta,1,1) = (1,1,1,...)$, thus $b_1(t;1,1,1) = b_1(t;\eta,1,1)$ given by (5.6). However, the two chains have different Δ_1, hence they have different memory functions given by (5.8) and (5.9), respectively.

Similarly, a *perfect* diatomic chain $(1,1,\lambda)$ and a diatomic chain with a *mass* impurity $(\eta,1,\lambda)$ share the same recurrants in S_1: $\sigma_1(1,1,\lambda) = \sigma_1(\eta,1,\lambda) = (1,1,\lambda,\lambda,1,1,\lambda,\lambda,...)$, thus they have same $b_1(t)$. Because of their different $\Delta_1(1,1,\lambda) = 2\lambda$ and $\Delta_1(\eta,1,\lambda) = 2\eta$, they have different memory functions given by (5.35a, b) and (5.36a, b), respectively.

On the other hand, we notice that only if a monatomic or a diatomic chain has a *full* impurity, has its $b_1(t)$ both pole and cut contributions, otherwise, the chain has cut contribution only, i.e.

$$b_1(t;\eta,\kappa,\lambda) = \begin{cases} b_1^{cut}(t;\eta,1,\lambda) & \text{if } \kappa = 1 \\ b_1^{pol}(t;\eta,\kappa,\lambda) + b_1^{cut}(t;\eta,\kappa,\lambda) & \kappa \neq 1 \end{cases}. \quad (5.37)$$

Conclusions

In this paper, the memory function of a *full* impurity in a diatomic chain is derived by means of the recurrence relations method. The memory function is contributed by poles and cuts. The former result in a cosine and the latter in acoustic and optic branches. Both branches are given by a convolution of a difference of two sines and an expansion of even-order Bessel functions. The expansion coefficients are integrals of elliptic function $sn(u)$ along the real axis in a complex plain for the acoustic branch, and integrals of elliptic function $nd(v)$ along a contour parallel to the imaginary axis in that plane for the optical branch, respectively.

Different special cases are examined and corresponding memory functions are derived. It turns out that a *perfect* monatomic chain and a monatomic chain with a *mass* impurity share the same $b_1(t)$, but their memory functions are different because of their different Δ_1. Same are true for diatomic chains. Besides, the memory function has pole contribution only if the chain has a *full* impurity, i.e. $\kappa \neq 1$.

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Appendix A

Now we derive general expressions (3.15a, b) based on calculation of the residues of function

$$h(z)=\frac{1}{2(\kappa-1)}\frac{(\kappa-2)z^3+p_1z+\kappa\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}}{(z^2+m^2)(z^2+n^2)}e^{zt} \quad \text{(A.1)}$$

at poles $\pm im$, $\pm in$ and on the signs of $D_m(\kappa,\lambda)$, $D_n(\kappa,\lambda)$ in different regions shown in Table 1.

Region III_d : $D_m(\kappa,\lambda)>0$ and $D_n(\kappa,\lambda)>0$. We have

$$\operatorname{Re}s\ h(im)=\frac{1}{2(\kappa-1)(-m^2+n^2)}\left[(\kappa-2)(-m^2)-p_1+\frac{\kappa}{im}(\pm i)\sqrt{(-m^2+a^2)(-m^2+b^2)(-m^2+c^2)}\right].$$

Recall (3.12), $\left[D_0(z)+zS(z)\right]_{z=im}=D_m(\kappa,\lambda)+im(\pm i)\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}=0$,

Since $D_m(\kappa,\lambda)>0$, we have to choose $S(im)=i\sqrt{\cdots}$. Thus

$$\operatorname{Re}s\ h(im)=\frac{1}{2(\kappa-1)(m^2-n^2)}\left[(\kappa-2)m^2-p_1-\frac{\kappa}{m}\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}\right]\frac{e^{imt}}{2}.$$

Similarly, residues of $h(z)$ at $-im$, $\pm in$ are obtained by choosing $S(-im)=-i\sqrt{\cdots}$, $S(in)=i\sqrt{\cdots}$ and $S(-in)=-i\sqrt{\cdots}$. Summing up the residues gives:

$$M=\frac{1}{2(\kappa-1)(m^2-n^2)}[(\kappa-2)m^2-p_1-\frac{\kappa}{m}\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}], \quad \text{(A.2a)}$$

$$N=\frac{1}{2(\kappa-1)(m^2-n^2)}[(2-\kappa)n^2+p_1+\frac{\kappa}{n}\sqrt{(n^2-a^2)(n^2-b^2)(n^2-c^2)}]. \quad \text{(A.2b)}$$

Set

$$M_1=\frac{(\kappa-2)m^2-p_1}{2(\kappa-1)(m^2-n^2)},\ M_2=\frac{\kappa\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}}{2(\kappa-1)(m^2-n^2)m};$$

$$N_1=\frac{(2-\kappa)n^2+p_1}{2(\kappa-1)(m^2-n^2)},\ N_2=\frac{\kappa\sqrt{(n^2-a^2)(n^2-b^2)(n^2-c^2)}}{2(\kappa-1)(m^2-n^2)n}.$$

Or by (2.13) ,

$$M_1=\frac{(\kappa-2)m^2-p_1}{4(\kappa-1)\Delta},\ M_2=\frac{\kappa\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}}{4(\kappa-1)\Delta m}; \quad \text{(A.3a)}$$

$$N_1=\frac{(2-\kappa)n^2+p_1}{4(\kappa-1)\Delta},\ N_2=\frac{\kappa\sqrt{(n^2-a^2)(n^2-b^2)(n^2-c^2)}}{4(\kappa-1)\Delta n}. \quad \text{(A.3b)}$$

It is able to show, especially easy to verify numerically that

$$M_1 = M_2,\; N_1 = N_2. \tag{A.4}$$

Thus in Region III_d the amplitudes are given by

$$M = M_1 - M_2 = 0, \tag{A.5a}$$

$$N = N_1 + N_2 = \frac{(2-\kappa)n^2 + p_1}{2(\kappa-1)\Delta} = \frac{\kappa\sqrt{(n^2-a^2)(n^2-b^2)(n^2-c^2)}}{2(\kappa-1)\Delta n}. \tag{A.5b}$$

Similarly, by the same considerations we obtain the amplitiutes *M* and *N* in different regions.

Region III_u: $D_m(\kappa,\lambda) < 0$ and $D_n(\kappa,\lambda) < 0$.

$$M = M_1 + M_2 = \frac{(\kappa-2)m^2 - p_1}{2(\kappa-1)\Delta} = \frac{\kappa\sqrt{(m^2-a^2)(m^2-b^2)(m^2-c^2)}}{2(\kappa-1)\Delta m}, \tag{A.6a}$$

$$N = N_1 - N_2 = 0. \tag{A.6b}$$

Region II_d: $D_m(\kappa,\lambda) > 0$ and $D_n(\kappa,\lambda) < 0$

$$M = M_1 - M_2 = 0, \tag{A.7a}$$

$$N = N_1 - N_2 = 0. \tag{A.7b}$$

Region II_u: $D_0(m) > 0$ and $D_0(n) > 0$.

$$M = M_1 - M_2 = 0, \tag{A.8a}$$

$$N = N_1 + N_2. \tag{A.8b}$$

Region I_d: $D_m(\kappa,\lambda) < 0$ and $D_n(\kappa,\lambda) < 0$.

$$M = M_1 + M_2, \tag{A.9a}$$

$$N = N_1 - N_2 = 0. \tag{A.9b}$$

Region I_u: $D_m(\kappa,\lambda) < 0$ and $D_n(\kappa,\lambda) < 0$.

$$M = M_1 + M_2, \tag{A.10a}$$

$$N = N_1 - N_2 = 0. \tag{A.10b}$$

Expressions (A.5) ~ (A.10) for M and N are indeed (3.15a, b).

Appendix B

In this appendix, we derive (5.23a, c).

B.1 By (5.22a),

$$U_0^{aou}(1,1,\lambda>1)=\int_0^{\pi/2}d\theta\sqrt{(1-l_1^2\sin\theta)(1-l_2^2\sin\theta)}\cos\theta\,. \tag{B.1}$$

Setting [32]

$$\sin^2\alpha=\frac{(1-l_2^2)\sin^2\theta}{1-l_2^2\sin^2\theta}, \tag{B.2}$$

we obtain

$$\cos\alpha d\alpha=\frac{(1-l_2^2)^{1/2}}{(1-l_2^2\sin^2\theta)^{3/2}}\cos\theta d\theta\,. \tag{B.3}$$

$$\sin^2\theta=\frac{\sin^2\alpha}{1-l_2^2\cos^2\theta},\ \cos\theta=\sqrt{\frac{1-l_2^2}{1-l_2^2\cos^2\alpha}}\cos\alpha\,, \tag{B.4}$$

$$1-l_1^2\sin^2\theta=(1-l_2^2)\frac{1-l^2\sin^2\alpha}{1-l_2^2\cos^2\alpha},\ l^2=\frac{l_1^2-l_2^2}{1-l_2^2}=\frac{1}{\lambda}<1\,, \tag{B.5}$$

$$1-l_2^2\sin^2\theta=\frac{1-l_2^2}{1-l_2^2\cos^2\alpha}\,. \tag{B.6}$$

With (B.3)-(B.6) we have

$$\frac{d\theta}{\sqrt{(1-l_1^2\sin^2\theta)(1-l_2^2\sin^2\theta)}}=\frac{1}{\sqrt{1-l_2^2}}\frac{d\alpha}{\sqrt{1-l^2\sin^2\alpha}}=\frac{1}{\sqrt{1-l_2^2}}du\,. \tag{B.7}$$

B.2 Write (B.1) as

$$U_0^{aou}(1,1,\lambda>1)=\int_0^{\pi/2}\frac{d\theta}{\sqrt{(1-l_1^2\sin^2\theta)(1-l_2^2\sin^2\theta)}}(1-l_1^2\sin^2\theta)(1-l_2^2\sin^2\theta)\cos\theta\,.$$

Substitution of (B.3)-(B.6) gives

$$U_0^{aco}(1,1,\lambda>1)=(1-l_2^2)^2\int_0^{K(l)}du\frac{cn(u,l)dn^2(u,l_2)}{[1-l_2^2cn^2(u,l_2)]^{5/2}}\,. \tag{B.8}$$

Similarly, make use of (5.5a),

$$U_n^{aou}(1,1,\lambda>1)=\int_0^{\pi/2}\frac{d\theta}{\sqrt{(1-l_1^2\sin^2\theta)(1-l_2^2\sin^2\theta)}}(1-l_1^2\sin^2\theta)(1-l_2^2\sin^2\theta)\cos\theta\left[1+\sum_{j=1}^{n}c_j(n)\sin^{2j}\theta\right]\cdot$$

Combining it with (B.3)-(B.6) leads to

$$U_n^{aco}(1,1,\lambda>1)=U_0^{aco}(1,1,\lambda>1)+\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(1,1,\lambda>1)\,, \quad \text{(B.9)}$$

$$\tilde{U}_j^{aco}(1,1,\lambda>1)=(1-l_2^2)^2\int_0^{K(l)}du\frac{cn(u,l)dn^2(u,l)sn^{2j}(u,l)}{[1-l_2^2cn^2(u,l)]^{j+5/2}}\,. \quad \text{(B.10)}$$

(B.8)- (B.10) give (5.23a, b, c).

Appendix C

In this appendix, we derive the expressions for the auxiliary integrals in optical branch.

In (5.26), introduce $sn(u)=\sin\alpha=r\sin\theta$ $(\sin\alpha_c=1,\ \sin\alpha_a=r>1)$, then

$$V_0^{opt}(1,1,\lambda<1)=\int_{\alpha_c}^{\alpha_a}\frac{d\alpha}{\sqrt{1-p^2\sin^2\alpha}}(1-p^2\sin^2\alpha)\cos^2\alpha\,,$$

Which may be written as

$$V_0^{opt}(1,1,\lambda<1)=p\int_{u_c}^{u_a}du\ cn^2(u,p)dn^2(u,p)\quad (p^2=1/r^2=\lambda/(\lambda+1)<1)\,. \quad \text{(C.1)}$$

By use of (5.5a, b),

$$V_n^{opt}(1,1,\lambda<1)=V_0^{opt}(1,1,\lambda<1)+\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(1,1,\lambda<1)\ \ (n=1,2,3,\ldots)\,, \quad \text{(C.2b)}$$

$$\tilde{V}_j^{opt}(1,1,\lambda<1)=p^{2j+1}\int_{u_c}^{u_a}du\ cn^2(u,p)dn^2(u,p)sn^{2j}(u,p)\,. \quad \text{(C.2c)}$$

At endpoints of the optical branch,

$$sn\ u_c=\sin\alpha_c=1/\sqrt{\lambda}>1\,,\ u_c=sn^{-1}(1/\sqrt{\lambda})\,, \quad \text{(C.3a)}$$

$$sn\ u_a=\sin\alpha_a=r=\sqrt{(\lambda+1)/\lambda}>1\,,\ u_a=sn^{-1}(\sqrt{(\lambda+1)/\lambda})\,. \quad \text{(C.3b)}$$

Hence u_c, u_a, are complex, and $sn(u,p)=sn(u+iv,p)$, $cn(u+iv,p)$, $dn(u+iv,p)$ are complex elliptic

functions. The integrals (C.1a, c) are carried out in a complex $u+iv$ plane. So

(C.3b) and (C.1 a, c) take the form

$$sn(u_a+iv_a,p)=\sin(\alpha_a+i\beta_a)=r>1\,, \quad \text{(C.4a)}$$

$$V_0^{opt}(1,1,\lambda<1)=p\int_{(u_c,v_c)}^{(u_a,v_a)}(du+idv)\ cn^2(u+iv,p)dn^2(u+iv,p)\,, \quad \text{(C.4b)}$$

$$\tilde{V}_j^{opt}(1,1,\lambda<1)=p^{2j+1}\int_{(u_c,v_c)}^{(u_a,v_a)}(du+idv)\ cn^2(u+iv.p)dn^2(u+iv,p)sn^{2j}(u+iv,p)\,. \quad \text{(C.4c)}$$

where $p' = \sqrt{1-p^2} < 1$ is the complementary modulus of p, and

$$v_c = sn^{-1}(\sqrt{1-\lambda^2}, p'). \tag{C.5}$$

By addition theorem [32], the complex elliptic functions may be replaced by real elliptic functions. With arguments similar to [18, especially in Appendix A], we obtain

$$V_0^{opt}(1,1,\lambda<1) = -ip(p')^4 \int_{v_c}^{K(p')} dv\ cd^2(v,p') sd^2(v,p'). \tag{C.6a}$$

$$\tilde{V}_j^{opt}(1,1,\lambda<1) = -ip^{2j+1}(p')^4 \int_{v_c}^{K(p')} dv\ cd^2(v,p') sd^2(v,p') nd^{2j}(v,p'), \tag{C.6b}$$

i.e. (5.27a, c). The contour $u = K(p)$ is parallel to the imaginary axis in the $u+iv$ plane.

By the same arguments, we have the auxiliary integrals for $\lambda > 1$ as

$$V_0^{opt}(1,1,\lambda>1) = -ip(p')^4 \int_0^{K(p')} dv\ cd^2(v.p') sd^2(v.p'), \tag{C.7a}$$

$$V_n^{opt}(1,1,\lambda>1) = V_0^{opt}(1,1,\lambda>1) + \sum_{j=1}^{n} c_j(n) p^{2j} \tilde{V}_j^{opt}(1,1,\lambda>1), \tag{C.7b}$$

$$\tilde{V}_j^{opt}(1,1,\lambda>1) = -ip^{2j+1}(p')^4 \int_0^{K(p')} dv\ cd^2(v,p') sd^2(v,p') nd^{2j}(v,p'), \tag{C.7c}$$

i.e. (5.33a, b)