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A Diatomic Chain with A Mass Impurity

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Abstract

A classic diatomic chain with one mass impurity is studied using the recurrence relations method. The momentum autocorrelation function of the impurity results from contributions of two pairs of resonant poles and three branch cuts. The pole contribution is given by cosine function(s) and the cut contribution is the acoustic and optical branches. The acoustic and optical branches are given by expansions of even-order Bessel function. The expansion coefficients are integrals of elliptic functions in the real axis in a complex plane for the acoustic branch and along a contour parallel to the imaginary axis for the optical branch, respectively. An integral $\int_0^{\varphi} d\theta/\sqrt{(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta)}$ $(r_2^2>r_1^2>1)$ *is evaluated.*

Introduction

It has a long history that harmonic oscillator chains are used as a model for solid state. Most of the early work used the normal coordinates method [1-4]. Since earlier 1980s, the recurrence relations method [5-8] is used in the study of various areas in physics [9-13] as well as in different models of oscillator chains [14-22].

The momentum autocorrelation function (ACF) of one impurity in a classic diatomic chain is studied using the recurrence relations (RR) method. It results from contributions of two pairs of resonant poles and three branch cuts [19]. The pole contribution is cosine function(s) and the cut contribution gives the acoustic and optical branches.

The cut contribution is derived as expansion of even-order Bessel functions by use of the convolution theorem. The expansion coefficients are integrals of real and complex elliptic functions for the acoustic and optical branches, respectively.

Because the elliptic function is greater than one at the lower end point of the optical branch cut, we encounter complex elliptic functions. The addition theorem helps reduce the complex elliptic function to a complex sum of two real ones. Hence the expansion coefficients are integrals of elliptic functions along the real axis in a complex plane for the acoustic branch and along a contour parallel to the imaginary axis for the optical branch , respectively.

By a special transformation, integral $\int_0^{\phi} d\theta/\sqrt{(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta)}$ is carried out where both r^2_1 and r^2_2 are greater than one.

Recurrence Relations Method

Let *A(t)* be a dynamical variable of a system governed by the Heisenberg's equations:

$$\frac{dA(t)}{dt}=\{A(t),H\}, \qquad (2.1)$$

where { , } is the Poisson bracket and Hamiltonian *H* is Hermitian. *A(t)* may be expamded as

$$A(t)=\sum_{\nu=0}^{d-1}a_\nu(t)f_\nu, \qquad (2.2)$$

where $\{f_\nu;\ \nu=0,1,2,....,d\text{-}1\}$ is a set of complete linearly independent orthogonal basis vectors spanning a realized space *S*, and $\{a_\nu(t)\}$ is a set of basis real functions bearing the time dependence of *A(t)*. $\{f_\nu\}$ are not necessarily normalized, and may depend on the properties of the inner product space such as temperature, chemical potentials, etc.

The norm or length of vector $A(t)$ is given by

$$\|A(t)\| = (A(t), A(t)), \qquad (2.3)$$

where *(A,B)* is the inner product of *A* and *B* being realizable according to the physical requirements of the model. In classic cases, the inner product is simply defined by the average of *AB*:

$$(A,B)=\prod_i\int dp_idq_ie^{-\beta H}AB/\prod_i\int dp_idq_i^{-\beta H}, \qquad (2.4)$$

where β is the inverse temperature. The realized space *S* has d dimensions and so does $A(t)$. d may be finite or denumerably infinite. For a Hermitian system, the norm of a dynamical vector $A(t)$ is a constant of motion: $\|A(t)\| = \|A\|$ [7].

If S is realized by inner product (2.4), then $\{f_\nu\}$ satisfy a set of three-term recurrence relations referred to as RR I:

$$f_{\nu+1} = Lf_\nu + \Delta_\nu f_{\nu-1}, \quad (\nu \geq 0, \quad f_{-1} = 0, \quad \Delta_0 \equiv 1), \qquad (2.5)$$

where $L \equiv \{\ ,H\}$ is the Liouvillian operator of the system,

$\Delta_\nu \equiv \|f_\nu\| / \|f_{\nu-1}\|$ and $\{\Delta_\nu\}$ is a set of recurrants.

Correspondingly, $\{a_\nu(z)\}$ also satisfy a set of three-term recurrence relations called RR II:

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t) \quad (a_{-1} \equiv 0, \quad 0 \leq \nu \leq d-1), \quad (2.6)$$

with $\dot{a}_\nu(t) = da_\nu(t)/dt$. The RR II is model-dependent.

The Laplace transform $L[\ a_0(t)\ ] = a_0(z)$ is related to the recurrants $\sigma = (\Delta_1 \Delta_2 \ldots, \Delta_{d-1})$ by a continued fraction:

$$a_0(z) = 1/(z + \Delta_1/(z + \Delta_2/z + \ldots \Delta_{d-1}/z)). \qquad (2.7)$$

If d is finite, the r.h.s. of (2.7) is a polynomial of finite order. In this case $a_0(t)$ is a periodic function. If $d \to \infty$, the r.h.s. of (2.7) is an infinite continued fraction.

The Model

Consider a diatomic chain composed of infinite classic oscillators. At sites $j_0 = \pm 1, \pm 3, \ldots$ locate oscillator m_1, at $j_e = \pm 2, \pm 4$ ... oscillator m_2 and at q_0 a mass impurity m_0. They interact with their nearest neighbours through Hook constant K under the periodic boundary conditions $q_{-N/2} = q_{N/2}$ and $p_{-N/2} = p_{N/2}$.

The Hamiltonian of the chain is given by

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

$$+ \cdots + (q_{-2} - q_{-1})^2 + (q_{-1} - q_0)^2]. \qquad (3.1)$$

The frequencies of the oscillators are defined by $\omega_i^2 = K/m_i$, $(i = 0,1,2)$. If choose $K = m_1 = 1$, then , $\omega_0^2 = \eta$, $\omega_1^2 = 1$ and $\omega_2^2 = \lambda$ where $\eta = m_1/m_0$ and $\lambda = m_1/m_2$ are parameters.

The recurrants are derived as [19]:

$$N \to \infty: \sigma = (2\eta, 1, 1\lambda.\lambda, 1, 1, \lambda.\lambda, 1, 1, \lambda.\lambda \ldots). \qquad (3.2)$$

Combining (3.2) with continued fraction (2.7) gives

$$a_0(z) = 1/z + 2\eta/A, \qquad (3.3)$$

where $A = z + 1/(z + 1/(z + \lambda/(z + \lambda/A)))$ is a quadratic equation for A, the solution is

$$A = \frac{1}{2(z^2 + \lambda + 1)}[z(z^2 + 2) + \sqrt{z^2(z^2 + 2)^2 + 4\lambda(z^2 + 2)(z^2 + \lambda + 1)}]$$

Substituting A into (3.3) yields [19]

$$a_0(z) = \frac{P(z) + S(z)}{D_0(z) + zS(x)}, \qquad (3.4)$$

where

$$P(z) = z(z^2 + 2), \qquad (3.5a)$$

$$S(z) = \sqrt{(z^2 + 2)(z^2 + 2\lambda)(z^2 + 2\lambda + 2)}, \qquad (3.5b)$$

$$D_0(z) = z^4 + 2(2\eta + 1)z^2 + 4\eta(\lambda + 1). \qquad (3.5c)$$

(3.4) can be rationalized as

$$a_0(z) = \frac{(\eta - \lambda)P(z) + \eta S(z)}{D(z)}, \qquad (3.6)$$

where

$$D(z) = (2\eta - \lambda)z^4 + 2(2\eta^2 + 2\eta - \lambda)z^2 + 4\eta^2(\lambda + 1), \qquad (3.7)$$

which may be factorized. Thus we obtain

$$a_0(z) = \frac{(1 - \alpha)P(z) + \alpha S(z)}{(z^2 + \mu^2)(z^2 + \nu^2)}, \qquad (3.8)$$

where

$$\mu^2 = \eta + 1 + \frac{\eta\lambda + \Delta}{2\eta - \lambda}, \qquad (3.9a)$$

$$\nu^2 = \eta + 1 + \frac{\eta\lambda - \Delta}{2\eta - \lambda}, \qquad (3.9b)$$

$$\Delta = \sqrt{4\eta^2(\eta - \lambda)^2 + (2\eta - \lambda)^2}, \qquad (3.9c)$$

$$\alpha = \frac{\eta}{2\eta - \lambda}. \qquad (3.10)$$

Now write $a_0(z)$ as $a_0(z;\eta,\lambda)$. Obviously, (3.8) has two pairs of resonant poles and three branch cuts shown in Fig. 1.

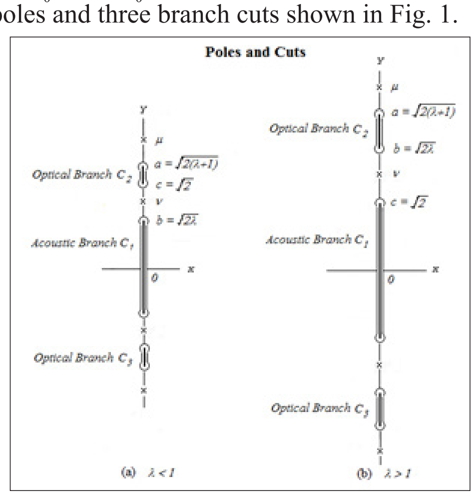

Figure 1: Poles ("x") and cuts (bold segment) of $a_0(z;\eta, \lambda)$

Completeting the inverse Laplace transform of (3.8) yields

$$a_0(t;\eta,\lambda) = a_0^{pol}(t:\eta,\lambda) + a_0^{cut}(t;\eta,\lambda), \qquad (3.11)$$

being contributions from the poles and cuts, respectively.

The cut contribution is a sum of acoustic and optical branches:

$$a_0^{cut}(t;\eta,\lambda) = a_0^{aco}(t:\eta,\lambda) + a_0^{opt}(t;\eta,\lambda). \qquad (3.12)$$

The initial condition of the momentum ACF reads

$$a_0(0;\eta,\lambda) = a_0^{pol}(0;\eta,\lambda) + a_0^{aco}(0;\eta,\lambda) + a_0^{opt}(0;\eta,\lambda) = 1 \cdot \qquad (3.13)$$

The Pole Contribution

Now introduce an $\eta - \lambda$ plane, in which line $\lambda = 1$ ($m_1 = m_2$) represents an equal mass chain with an impurity; line $\eta = \lambda$ ($m_0 = m_2$) gives a diatomic chain; and intersection of the two lines ($m_0 = m_1 = m_2$) represents a monatomic chain, etc. These two lines divide the plane into four regions I_d, I_u, II_u and II_d shown in Figure 2.

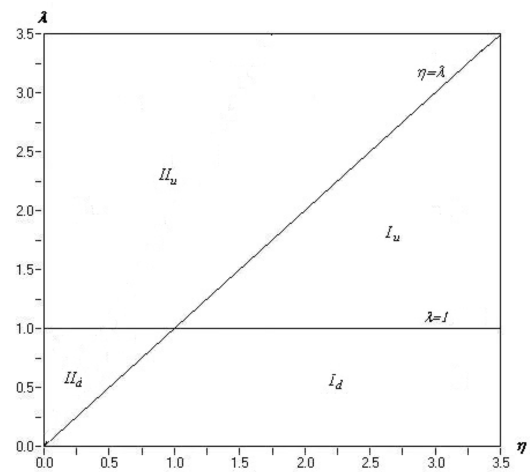

Figure 2: Regions I_d, I_u, II_u and II_d and in the $\eta - \lambda$ plane

It is easy to verify that

$b < v < c < a < \mu$, ($\lambda < 1$), $c \le v \le b < a < \mu$ ($\lambda \ge 1$). (4.1)

The pole contribution is given by [19]

$$a_0^{pole}(t;\eta,\lambda) = \begin{cases} M\cos\mu t + N\cos\nu t, & I_d \quad (m_2 > m_1, m_0) \\ M\cos\mu t & I_u \quad (m_1 > m_2 > m_0) \\ N\cos\nu t, & II_u \quad (m_0, m_1 > m_2) \\ 0, & II_p \quad (m_0 > m_2 > m_1) \end{cases}. \qquad (4.2)$$

It shows that region I_d is the physical region for both mode μ and v; I_u is the physical region for μ only; II_u is for mode v only; and II_d is not physical for both μ, v.

The frequencies μ, v are determined by (3.7) and the amplitudes M, N are derived as

$$M(\eta,\lambda) = \frac{\eta-\lambda}{\Delta}(\mu^2 - c^2), \quad N(\eta,\lambda) = \frac{\eta-\lambda}{\Delta}(c^2 - \nu^2). \qquad (4.3)$$

(4.3) is valid in all four regions. It is also valid in the limits $\lambda \to 0$ and ∞; while it is valid for N but not for M when $\eta \to 0$ ($m_0 \to \infty$) and ∞ ($m_0 \to 0$) [21].

Contribution of Cuts

Now consider the cut contribution. Since $P(z)$ is odd in z, by (3.8) we have

$$a_0^{aco}(t;\eta,\lambda<1) = \frac{2\alpha}{\pi}\int_0^b dy \frac{\sqrt{(a^2-y^2)(b^2-y^2)(c^2-y^2)}}{(\mu^2-y^2)(\nu^2-y^2)}\cos yt, \qquad (5.1a)$$

$$a_0^{aco}(t;\eta,\lambda>1) = \frac{2\alpha}{\pi}\int_0^c dy \frac{\sqrt{(a^2-y^2)(b^2-y^2)(c^2-y^2)}}{(\mu^2-y^2)(\nu^2-y^2)}\cos yt; \qquad (5.1b)$$

$$a_0^{opt}(t;\eta,\lambda<1) = \frac{2\alpha}{\pi}\int_c^a dy \frac{\sqrt{(a^2-y^2)(b^2-y^2)(c^2-y^2)}}{(\mu^2-y^2)(\nu^2-y^2)}\cos yt, \qquad (5.2a)$$

$$a_0^{opt}(t;\eta,\lambda>1) = \frac{2\alpha}{\pi}\int_b^a dy \frac{\sqrt{(a^2-y^2)(b^2-y^2)(c^2-y^2)}}{(\mu^2-y^2)(\nu^2-y^2)}\cos yt. \qquad (5.2b)$$

Generally, it is not easy to carry out the inverse Laplace transform of (3.8). If write it as $a_0(z) = f(z)g(z)$, the convolution theorem allows us to carry out the inverse Laplace transforms separately:

$$F(t) = \mathrm{L}^{-1}[f(z)], \quad G(t) = \mathrm{L}^{-1}[g(z)], \text{ and}$$

$$a_0(t) = \int_0^t d\tau F(t-\tau)G(\tau) = \int_0^t d\tau F(\tau)G(t-\tau). \qquad (5.3)$$

We choose

$$f(z) = \frac{1}{(z^2+\mu^2)(z^2+\nu^2)},$$

$$g(z) = \alpha\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)},$$

than [23,24(a)]

$$F(t) = \frac{\mu\sin\nu t - \nu\sin\mu t}{\mu\nu(\mu^2-\nu^2)},$$

$$G(t) = \frac{\alpha}{2\pi i}\oint_C dz\sqrt{(z^2+a^2)(z^2+b^2)(z^2+c^2)}e^{zt}.$$

Acoustic Branch

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

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

By $y = b\sin\Theta$ ($\sin\Theta_b = 1$) and

$$\cos(bt\sin\theta)=J_0(bt)+2\sum_{n=1}^{\infty}J_{2n}(bt)\cos(2n\theta), \qquad (5.4)$$

we have

$$G^{aco}(t;\eta,\lambda<1)=\frac{2\alpha ab^2c}{\pi}[U_0^{aco}(\lambda<1)J_0(bt)$$

$$+2\sum_{n=1}^{\infty}U_n^{aco}(\lambda<1)J_{2n}(bt)], \qquad (5.5)$$

where

$$U_n^{aco}(\lambda<1)=\int_0^{\pi/2}d\theta\cos^2\theta\sqrt{(1-k_1^2\sin^2\theta)(1-k_2^2\sin^2\theta)}\cos(2n\theta)$$

$$(n=0,1,2....), \qquad (5.6)$$

are auxillary integrals; and

$k_1^2 = (b/c)^2 = \lambda<1$, $k_2^2 = (b/a)^2 = \lambda/(\lambda+1)$, $k_2^2 < k_1^2$ (5.7)

are parameters.

Make use of [25(a)] and set [25(b)]

$$R(\sin^2\theta)=(1-\sin^2\theta)(1-k_1^2\sin^2\theta)(1-k_2^2\sin^2\theta),$$

then

$$U_0^{aco}(\lambda<1)=\int_0^{\pi/2}d\theta\cos^2\theta\sqrt{(1-k_1^2\sin^2\theta)(1-k_2^2\sin^2\theta)}$$

$$=g_k\int_0^{K(k)}du[1-\frac{sn^2(u,k)}{1-k_2^2cn^2(u,k)}][1-\frac{k_1^2sn^2(u,k)}{1-k_2^2cn^2(u,k)}][1-\frac{k_2^2sn^2(u,k)}{1-k_2^2cn^2(u,k)}]$$

where $g_k=1/\sqrt{1-k_2^2}$, $k=\sqrt{(k_1^2-k_2^2)/(1-k_2^2)}=\lambda<1$

is the modulus and $K(k)$ the complete Legendre elliptic integral of the first kind. It can be expanded and evaluated as [22]

$$U_0^{aco}(\lambda<1)=g_k\sum_{m=0}^{3}(-1)^m\frac{C_m(\lambda<1)}{(1-k_2^2)^m}\int_0^{K(k)}du[\frac{sn^2(u,k)}{1-\alpha_k^2sn^2(u,k)}]^m, \qquad (5.8)$$

where $\alpha_k^2 = k_2^2/(k_2^2-1)>1$ is a parameter ($\alpha_k^2 \neq 1$ or k^2); by (5.7), the coefficients are given by

$$C_0(\lambda<1)=1,\quad C_1(\lambda<1)=(\lambda^2+3\lambda+1)/(\lambda+1),$$

$$C_2(\lambda<1)=2\lambda,\quad C_3(\lambda<1)=\lambda^2/(\lambda+1); \qquad (5.9)$$

and

$$I_m^{aco}(\lambda<1)=\int_0^{K(k)}du[\frac{sn^2(u,k)}{1-k_2^2cn^2(u,k)}]^m \quad (m=0,1,2,3). \qquad (5.10)$$

Further, (5.8) can be evaluated as

$$U_0^{aco}(\lambda<1)=\frac{g_k}{4\lambda}[(8\lambda^2+24\lambda+7)K(k)+E(k)+2\lambda\Pi(\alpha_k^2,k)],$$

given in terms of complete Legendre elliptic integrals of the first, second and third kinds.

Similarly,

$$U_n^{aco}(\lambda<1)=\int_0^{\pi/2}d\theta\cos^2\theta\sqrt{(1-k_1^2\sin^2\theta)(1-k_2^2\sin^2\theta)}\cos(2n\theta)$$

$$(n=1,2,3....). \qquad (5.11)$$

Make use of [24(b)]

$$\cos(2n\theta)=1+\sum_{j=1}^{n}c_j(n)\sin^{2j}\theta, \qquad (5.12a)$$

$$c_1=-\frac{4n^2}{2!},\quad c_2=\frac{4n^2(4n^2-2^2)}{4!},$$

$$c_3=-\frac{4n^2(4n^2-2)(4n^2-4^2)}{6!},\quad \ldots, \qquad (5.12b)$$

then (5.11) reads

$$U_n^{aco}(\lambda<1)=U_0^{aco}(\lambda<1)+\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda<1)\quad (n=1,2,3,...), \qquad (5.13)$$

where

$$\tilde{U}_j^{aco}(\lambda<1)=\int_0^{\pi/2}d\theta\cos^2\theta\sqrt{(1-k_1^2\sin^2\theta)(1-k_2^2\sin^2\theta)}\sin^{2j}\theta, \qquad (5.14a)$$

it can be evaluate and expand as [22]

$$\tilde{U}_j^{aco}(\lambda<1)=g_k\sum_{m=0}^{3}(-1)^m\frac{C_m(\lambda<1)}{(1-k_2^2)^{j+m}}\int_0^{K(k)}du[\frac{sn^2(u,k)}{1-\alpha_k^2sn^2(u,k)}]^{j+m}.$$

Thus (5.5) takes the form

$$G^{aco}(t;\eta,\lambda<1)=\frac{2\alpha ab^2c}{\pi}[U_0^{aco}(\lambda<1)$$

$$+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda<1)J_{2n}(bt)]. \quad (5.15)$$

where $J_0(bt)+2\sum_{n=1}^{\infty}J_{2n}(bt)=1$ is used.

Therefore the acoustic branch is given by

$$a_0^{aco}(t;\eta,\lambda<1)=\frac{2\alpha ab^2c}{\pi\mu\nu(\mu^2-\nu^2)}\int_0^t d\tau[\mu\sin(\nu\tau)-\nu\sin(\mu\tau)]\times$$

$$[U_0^{aco}(\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda<1)J_{2n}(bt-b\tau)]. \quad (5.16)$$

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

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

Similarly, set $y=c\cos\Theta$ ($\sin\Theta_c=1$), we obtain the acoustic branch

$$a_0^{aco}(t;\eta,\lambda>1)=\frac{2\alpha abc^2}{\pi\mu\nu(\mu^2-\nu^2)}\int_0^t d\tau[\mu\sin(\nu\tau)-\nu\sin(\mu\tau)]\times$$

$$[U_0^{aco}(\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{U}_j^{aco}(\lambda>1)J_{2n}(ct-c\tau)], \quad (5.17)$$

where

$$U_0^{aco}(\lambda>1)=g_l\sum_{m=0}^{3}(-1)^m\frac{C_m(\lambda>1)}{(1-l_2^2)^m}\int_o^{K(l)}du[\frac{sn^2(u,l)}{1-\alpha_l^2sn^2(u,l)}]^m, \quad (5.18)$$

$$\tilde{U}_j^{aco}(\lambda>1)=g_l\sum_{m=0}^{3}(-1)^m\frac{C_m(\lambda>1)}{(1-l_2^2)^{j+m}}\int_o^{K(l)}du[\frac{sn^2(u,l)}{1-\alpha_l^2sn^2(u,l)}]^{j+m}, \quad (5.19)$$

$$C_0(\lambda>1)=1,\ C_1(\lambda>1)=(3\lambda+2)/\lambda(\lambda+1),$$

$$C_2(\lambda>1)=2/\lambda,\ C_3(\lambda>1)=1/\lambda(\lambda+1), \quad (5.20)$$

are coefficients; $g_l=1/\sqrt{1-l_2^2}$, $l=\sqrt{(l_1^2-l_2^2)/(1-l_2^2)}=1/\lambda<1$

is the modulus; and $\alpha_l^2=-l_2^2/(1-l_2^2)=-\lambda<0$ $(\alpha_l^2\ne 1$ or $l^2)$,

$l_1^2=(c/b)^2=1/\lambda<1$, $l_2^2=(c/a)^2=1/(\lambda+1)<1$, $l_2^2<l_1^2$ are parameters.

Also, U_0^{aco} ($\lambda>1$) can be expressed in terms of complete Legendre elliptic integrals of the first, second and third kinds:

$$U_0^{aco}(\lambda>1)=g_l[-\frac{5\lambda^2+24\lambda+20}{4\lambda}K(l)+\frac{\lambda}{4}E(l)+\frac{5\lambda+4}{2\lambda}\Pi(\alpha_l^2,l)].$$

In (5.16) or (5.17), the acoustic branch is expressed as even-order Bessel function expansion, the expansion coefficients are integrals of elliptic functions. The auxillary integral U_0^{aco} may be expressed in terms of Legendre elliptic integrals of the first, second and third kinds.

Optical Branch

Now consider the optical branch with different values of λ.

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

$$G^{opt}(t;\eta,\lambda<1)=\frac{2\alpha}{\pi}\int_c^a dy\sqrt{(a^2-y^2)(b^2-y^2)(c^2-y^2)}\cos(yt).$$

By $y=a\sin\Theta$, ($\sin\gamma=c/a$) and (5.4), it becomes

$$G^{opt}(t;\eta,\lambda<1)=\frac{2\alpha a^2bc}{\pi}[V_0^{opt}(\lambda<1)J_0(at)+2\sum_{n=1}^{\infty}V_n^{opt}(\lambda<1)J_{2n}(at)]. \quad (5.21)$$

The auxillary integrals are defined by

$$V_n^{opt}(\lambda<1)=\int_\gamma^{\pi/2}d\theta\cos^2\theta\sqrt{(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta)}\cos(2n\theta)$$

(n=0,1,2...), (5.22)

$$r_1^2=(a/c)^2=\lambda+1>1,\ r_2^2=(a/b)^2=(\lambda+1)/\lambda>1,$$

$$r_2^2>r_1^2>1. \quad (5.23)$$

Consider

$$V_0^{opt}(\lambda<1)=\int_\gamma^{\pi/2}d\theta\cos^2\theta\sqrt{(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta)}. \quad (5.24)$$

It is different from (5.6) because $r_2^2>r_1^2>1$. Using $\sin^2\varphi=[(r_2^2-1)/(r_2^2\sin^2\theta-1)]\sin^2\theta$ and setting

$$R(\sin^2\theta)=(1-\sin^2\theta)(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta),$$

we obtain [22]

$$V_0^{opt}(\lambda<1)=ig_r\int_{u_c}^{u_a}du[1-\frac{sn^2(u,\kappa_r)}{1-r_2^2cn^2(u,\kappa_r)}]\times$$

$$[1-r_1^2\frac{sn^2(u,\kappa_r)}{1-r_2^2cn^2(u,\kappa_r)}][1-r_2^2\frac{sn^2(u,\kappa_r)}{1-r_2^2cn^2(u,\kappa_r)}],$$

where $g_r=1/\sqrt{r_2^2-1}$ and $\kappa_r=\sqrt{(r_2^2-r_1^2)/(r_2^2-1)}=\sqrt{1-\lambda^2}<1$ a modulus. Further, it can expanded as

$$V_0^{opt}(\lambda<1)=ig_r\sum_{m=0}^{3}\frac{C_m(\lambda)}{(r_2^2-1)^m}\int_{u_c}^{K_r}du[\frac{sn^2(u,\kappa_r)}{1-\alpha_r^2sn^2(u,\kappa_r)}]^m. \tag{5.25}$$

The expansion coefficients are

$$C_0(\lambda)=1,\ C_1(\lambda)=(\lambda^2+3\lambda+1)/\lambda,$$
$$C_2(\lambda)=2(\lambda+1)^2/\lambda,\ C_3(\lambda)=(\lambda+1)^2/\lambda; \tag{5.26}$$

and parameter $\alpha_r^2=r_2^2/(r_2^2-1)>1$ but $\neq 1$ or k_r^2. The limits of integration are determined by

$$K_r\equiv K(\kappa_r),\quad u_c=sn^{-1}(1/\kappa_r)=sn^{-1}(1/\sqrt{1-\lambda^2})>1. \tag{5.27}$$

Similarly,

$$V_n^{opt}(\lambda<1)=\int_\gamma^{\pi/2}d\theta\cos^2\theta\sqrt{(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta)}\cos(2n\theta)$$
$$(n=1,2,...) \tag{5.28}$$

By (5.12), (5.28) is evaluated and expanded as [22]

$$V_n^{opt}(\lambda<1)=V_0^{opt}(\lambda<1)+\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda<1), \tag{5.29}$$

$$\tilde{V}_j^{opt}(\lambda<1)=ig_r\sum_{m=0}^{3}(-1)^j\frac{C_m(\lambda)}{(r_2^2-1)^{j+m}}\int_{u_c}^{u_a}du[\frac{sn^2(u,\kappa_r')}{1-\alpha_r^2sn^2(u,\kappa_r')}]^{j+m}. \tag{5.30}$$

However, by (5.27), $sn\,u_c=1/\kappa_r>1$, so u_c, $sn(u_c,\kappa_r)$ and $sn(u,\kappa_r)$ are complex. Hence the integral in (5.25) takes the form

$$[\int_{u_c}^{K(\kappa_r)}du+i\int_{v_c}^{v_a}dv][\frac{sn^2(u+iv,\kappa_r)}{1-\alpha_r^2sn^2(u+iv,\kappa_r)}]^m.$$

By the addition theorem [26] and $sn(u+iv,\kappa_r)\geq 1$ being real, we have $u=K(\kappa_r)$ and $sn(u+iv,\kappa_r)$ replaced by $nd(v,\kappa_r')$ [17,18] where nd is a Jacobian elliptic function, $\kappa_r'=\sqrt{1-\kappa_r^2}$ is a complementary modulus.

Since $u=K(\kappa_r)$ is a constant, $du=0$, so (5.25) and (5.30) become

$$V_0^{opt}(\lambda<1)=-g_r\sum_{m=0}^{3}\frac{C_m(\lambda)}{(r_2^2-1)^m}\int_{v_c}^{v_a}dv[\frac{nd^2(v,\kappa_r')}{1-\alpha_r^2nd^2(v,\kappa_r')}]^m, \tag{5.31}$$

$$\tilde{V}_j^{opt}(\lambda<1)=-g_r\sum_{m=0}^{3}(-1)^j\frac{C_m(\lambda)}{(r_2^2-1)^{j+m}}\int_{v_c}^{v_a}dv[\frac{nd^2(v,\kappa_r')}{1-\alpha_r^2nd^2(v,\kappa_r')}]^{j+m}. \tag{5.32}$$

The limits of integration are given by

$$v_a=nd^{-1}(1,\kappa_r'),\ \ v_c=nd^{-1}(1/\kappa_r,\kappa_r')=nd^{-1}(1/\sqrt{1-\lambda^2},\kappa_r'). \tag{5.33}$$

Substituting (5.31), (5.29) and (5.32) into (5.21) gives

$$G^{opt}(t;\eta,\lambda<1)=\frac{2\alpha a^2bc}{\pi}[V_0^{opt}(\lambda<1)J_0(at)$$
$$+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda<1)J_{2n}(at)]. \tag{5.34}$$

Therefore, the optical branch is given by

$$a_0^{opt}(t;\eta,\lambda<1)=\frac{2\alpha a^2bc}{\pi\mu\nu(\mu^2-\nu^2)}\int_0^t d\tau[\mu\sin(\nu\tau)-\nu\sin(\mu\tau)]\times$$

$$[V_0^{tpt}(\lambda<1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda<1)J_{2n}(at-a\tau)]. \tag{5.35}$$

For $\lambda>1$ $(0<c<b\leq y\leq a)$,

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

By similar arguments, we obtain

$$a_0^{opt}(t;\eta,\lambda>1)=\frac{2\alpha a^2bc}{\pi\mu\nu(\mu^2-\nu^2)}\int_0^t d\tau[\mu\sin(\nu\tau)-\nu\sin(\mu\tau)]\times$$

$$[V_0^{opt}(\lambda>1)+2\sum_{n=1}^{\infty}\sum_{j=1}^{n}c_j(n)\tilde{V}_j^{opt}(\lambda>1)J_{2n}(at-a\tau)], \tag{5.36}$$

where

$$V_0^{opt}(\lambda>1)=-g_s\sum_{m=0}^{3}\frac{C_m(\lambda)}{(s_2^2-1)^m}\int_{v_b}^{v_a}dv[\frac{nd^2(v,\kappa_s')}{1-\alpha_s^2nd^2(v,\kappa_s')}]^m, \tag{5.37}$$

$$\tilde{V}_j^{opt}(\lambda > 1) = -g_s \sum_{m=0}^{3} (-1)^j \frac{C_m(\lambda)}{(s_2^2 - 1)^{j+m}} \int_{v_b}^{v_a} dv \left[\frac{nd^2(v, \kappa_s')}{1 - \alpha_s^2 nd^2(v, \kappa_s')}\right]^{j+m}, \quad (5.38)$$

the coefficients $C_m(\lambda)$ are still given by (5.26); $g_s = 1/\sqrt{s_2^2 - 1}$,

$\kappa_s' < 1$ is complementary to modulus

$$\kappa_s = \sqrt{(s_2^2 - s_1^2)/(s_2^2 - 1)} = \sqrt{\lambda^2 - 1}/\lambda < 1;$$

$\alpha_s^2 = [s_2^2/(s_2^2 - 1)] = (\lambda + 1)/\lambda > 1$ but $\neq 1$ or κ_s^2, being a parameter; $s_1^2 = (a/b)^2 = (\lambda+1)/\lambda > 1$, $s_2^2 = (a/c)^2 = \lambda + 1 > 1$,

$s_2^2 > s_1^2$ are parameters.

In (5.35) or (5.36), the optical branch is an even-order Bessel function expansion, the expansion coefficients are integrals of elliptic functions along a contour parallel to the imaginary axis in a complex $u+iv$ - plane.

Modulus Relations

By the definitions of k, l, κ_r, κ_s we find that

$$\begin{aligned} k^2 + \kappa_r^2 &= 1, \\ l^2 + \kappa_s^2 &= 1; \end{aligned} \quad \text{or} \quad \begin{aligned} k &= \kappa_r', \\ l &= \kappa_s'. \end{aligned} \quad \text{if} \quad \begin{aligned} &\lambda < 1, \\ &\lambda > 1. \end{aligned} \quad (5.39)$$

Thus we have the modulus relations:

The moduluses of the elliptic functions in the expansion coefficients of the acoustic and optical branches are complementary one to another.

Besides, by $K(\kappa) = K'(\kappa')$, etc. and (5.39), we have

$$K(k) = K'(\kappa_r), \; K(l) = K'(\kappa_s). \quad (5.40)$$

The values of the upper integration limits in the coefficients of acoustic and optical branches are equal.

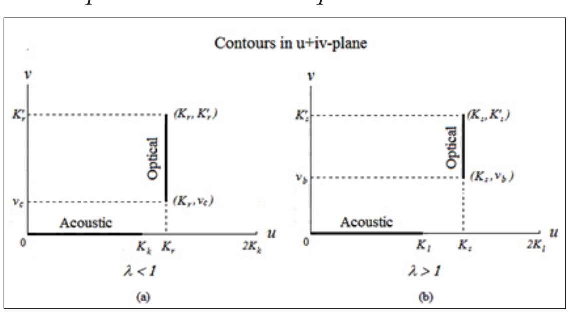

Figure 3: Integration contours in the $u+iv$ - plane

(a) For Eqs.(5.18) and (5.38) with $\lambda<1$.
(b) For Eqs.(5.19) and (5.39) with $\lambda>1$.

Conclusions

We have derived the momentum ACF of the impurity in a diatomic chain. The pole contribution is cosine function(s). General expressions for the frequencies and amplitudes are derived. In different regions in the η - λ -plane, the two resonant modes μ and v may exist simultaneously, only one or none, depending upon the values of (η, λ).

The acoustic and optical branches are derived as expansions of even-order Bessel functions. The expansion coefficients are integrals of real and complex elliptic functions for the acoustic and optical branches, respectively. The addition theorem helps deal with the complex elliptic function.

Therefore the expansion coefficients are given by integrals of elliptic functions along the real axis in a complex plane for acoustic branch and that along a contour parallel to the imaginary axis for optical branch, respectively. Besides, auxillary integrals $U_0^{aco}(\lambda)$ can be expressed in terms of complete Legendre elliptic integrals of the first, second and third kind. The time range is confined to t >0.

The derived pole and cut contributions present deeper insight to the momentum autocorrelation function of the impurity in a classic diatomic chain.

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