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A complex approximation method for differential equation systems describing a chain of interacting oscillations in crystals including spin waves

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Dedicated to memory of Professor Promarz M. Tamrazov

The system of differential equations of the form

$$\frac{d^2}{dt^2}x_r = \begin{cases} \omega^2(x_2 - x_1) + \kappa_1 \quad \text{for} \quad r = 1, \\ \omega^2(x_{r+1} - 2x_r + x_{r-1}) + \kappa_r \quad \text{for} \quad r = 2, 3, ..., n-1, \\ -\omega^2(x_n - x_{n-1}) + \kappa_n \quad \text{for} \quad r = n. \end{cases} \qquad (0)$$

is discussed with $\omega \in \mathbb{R}^+$ and κ_r being $\mathbb{R}$-valued continuous functions. With help of a complex approximation method the functions x_r are approached by finite sums involving convolutions of Bessel functions and the functions κ_r. Since we may let (x_r) correspond to consecutive atom sites (including empty sites) in a chain of crystallographic lattice, transversal to the surface, mathematically, our solution relates also the general solution to the solution for a fixed leaf of a foliation generated by layers of the crystal in question, in our case the third leaf from the boundary surface.
Physically, the result, extending those of R. W. Zwanzig (1960), A. S. Dolgov and N. A. Khizhnyak (1969), J. B. Sokoloff (1990), and B. Gaveau, J. Ławrynowicz and L. Wojtczak (1994, 2005, 2009), permits including in interacting oscillations the dependence on spin waves.

1. Introduction and motivation. The theme is somehow related to two research activities of our unforgetable friend Professor Promarz M. Tamrazov [1]:

- difference and differential contour-solid problems for holomorphic (and meromorphic) functions in the complex plane and in complex analytic spaces,
- equilibrium potentials of general condensers and their complete description (in our case this corresponds to the so-called *stochiometric,* entropy depending configurations of atoms and vacancies in sites of the crystallographic lattice).

We consider a system of equations (0) with $\omega \in \mathbb{R}^+$ and x_r being $\mathbb{R}$-valued continuous functions. The equations (0) are simplified by introducing the following substitutions and new units:

$$\begin{cases} \omega^2 K \widetilde{u}_{2r}(\tau) = 2\,(d/d\tau)\,x_r(\tau) \quad \text{for } r = 1, \dots, n, \\ \omega^2 K \widetilde{u}_{2r+1}(\tau) = x_r(\tau) - x_{r+1}(\tau) \quad \text{for } r = 1, \dots, n-1, \\ \omega^2 K \widetilde{u}_{2n+1}(\tau) = x_n(\tau), \quad \tau = 2\omega t \ \text{ and } \ \omega = \sqrt{K/m}, \end{cases} \tag{1}$$

m standing for the mass of all (identical) atoms and K denoting the lattice force constant. An easy calculation shown that the substitutions (1) into (0) give the system

$$\begin{cases} \dfrac{d}{d\tau}\widetilde{u}_2(\tau) = -\dfrac{1}{2}\left[\widetilde{u}_3(\tau) - \varepsilon_1\right], \\ \dfrac{d}{d\tau}\widetilde{u}_r(\tau) = \dfrac{1}{2}\left[\widetilde{u}_{r-1}(\tau) - \widetilde{u}_{r+1}(\tau) + \varepsilon_{\frac{1}{2}r}\right] \text{ for } r = 4, 6, ..., 2n-2, \\ \dfrac{d}{d\tau}\widetilde{u}_r(\tau) = \dfrac{1}{2}\left[\widetilde{u}_{r-1}(\tau) - \widetilde{u}_{r+1}(\tau)\right] \text{ for } r = 3, 5, ..., 2n-3, \\ \dfrac{d}{d\tau}\widetilde{u}_{2n}(\tau) = \dfrac{1}{2}\left[\widetilde{u}_{2n-1}(\tau) + \varepsilon_r\right], \\ \dfrac{d}{dt}\widetilde{u}_{2n+1}(\tau) = \dfrac{1}{2}\widetilde{u}_{2n}(\tau), \ \varepsilon_r = \left[1/\omega^4 K\right]\kappa_r \text{ and } \omega^4 K \neq 0. \end{cases} \tag{2}$$

The first differential equation in (2), because of the explicit appearance of $\widetilde{u}_3$ in it, showns the specific role of the third layer. We rewrite the system of equations (2) in a more convenient form. Let $u_r = u_r(\tau) = \widetilde{u}_{r+2}(\tau)$ for $r = 0, ..., 2n-2$. Then (2) becomes

$$\begin{cases} \dfrac{d}{d\tau}u_0 = -\dfrac{1}{2}\left(u_1 - \varepsilon_1\right), \\ \dfrac{d}{d\tau}u_r = \dfrac{1}{2}\left(u_{r-1} - u_{r+1} + \varepsilon_{\frac{1}{2}r+1}\right) \text{ for } r = 2, 4, \ldots, 2n-4, \\ \dfrac{d}{d\tau}u_r = \dfrac{1}{2}(u_{r-1} - u_{r+1}) \text{ for } r = 1, 3, \ldots, 2n-3, \\ \dfrac{d}{d\tau}u_{2n-2} = \dfrac{1}{2}(u_{2n-3} + \varepsilon_n), \\ \dfrac{d}{d\tau}u_{2n-1} = \dfrac{1}{2}u_{2n-2}. \end{cases} \tag{3}$$

We have to suppose that $\varepsilon_1, \varepsilon_2, ..., \varepsilon_n$ are $\mathbb{R}$-valued continuous functions. In addition to $u_1 = \widetilde{u}_3$ *also* $u_3 = \widetilde{u}_5$ *has a specific role*, analogous to that of u_3 in [2] — we can express $(d^2/d\tau^2)u_1$ as a linear function of u_3:

$$\begin{aligned} \frac{d^2}{d\tau^2}u_1 = \frac{1}{2}\left(\frac{d}{d\tau}u_0 - \frac{d}{d\tau}u_2\right) &= \frac{1}{4}(u_1 - \varepsilon_1) - \frac{1}{4}(u_1 - u_3 + \varepsilon_2) = \\ &= \frac{1}{4}(u_3 - \varepsilon_1 - \varepsilon_2). \end{aligned} \tag{4}$$

We summarize with the following

Key Lemma. *The substitutions* (1) *give rise to replace the system* (0) *by the system of first order differential equations* (3) *with* ε_r *being nonvanishing* $\mathbb{R}$*-valued functions and the equation for* $r = 1$ *replaced by the second order equation* (4).

The role of the above mentioned replacement and a possibility of using some u_{r_0} instead of u_1 have been discussed in detail in [2]; cf. also the beginning of Section 2 and Theorem 1. Physical applications of the results presented in the Key Lemma, the Extended Third-Layer Theorem given in Section 2, and the Extended k th-Layer Theorem given in Section 3 will be published in [3], focusing on lattice interaction dynamics and thermodynamical chaos; applications related with thermodynamical spin wave description — [4]; for an earlier physical content see [2, 5 — 10]. Further results relates with [3], in the context of composition algebras will appear in [11].

2. Extended Third-Layer Theorem. The equation (4) plays the key role in the problem of solving the system of (3), $r \neq 1$, and (4). Indeed, we can extended the Third-Layer Theorem of [7, 2] as follows:

Theorem 1. *For the sake of simplicity confine ourselves to the case*

$$u_0 = u_2,\ u_1 = u_3,\ u_{2n-2} = u_{2n-4},\ u_{2n-1} = u_{2n-3}. \tag{5}$$

The function $u_3 = u_3(\tau)$ *in the solution*

$$u_k = u_k(\tau),\ k = 1, 2, ..., 2n-1, \tag{6}$$

of the system of (3), $r \neq 1$, *and* (4) *can be expressed as*

$$u_3(t) = -\int_0^t \frac{2}{t-s} J_2(t-s) u_1(s) ds +$$

$$+ \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \int_0^t \Big[\frac{r}{t-s} J_r(t-s) - \frac{r-2}{t-s} J_{r-2}(t-s) \Big] \varepsilon_{\frac{1}{2}r+1}(s) ds -$$

$$-2 \sum_{r=0}^{2n-1} (-1)^r \left[\frac{r}{t} J_r(t) - \frac{r-2}{t} J_{r-2}(t) \right] u_r(0), \tag{7}$$

where $J_r,\ r = 0, 1, ...,$ *are the Bessel functions of the first kind.*

Proof. Let us consider the generating function

$$\Theta(z, \tau) = \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} u_r(\tau) z^r + \sum_{\substack{r=1,\\ r \text{ odd}}}^{2n-1} u_r(\tau) z^r,$$

for $z \in \mathbb{C},\ \tau \in [0, \tau^*]$. By (3) it satisfies the relation

$$2 \frac{\partial}{\partial \tau} \Theta = -(u_1 - \varepsilon_1) + \sum_{\substack{r=1,\\ r \text{ odd}}}^{2n-1} u_r z^{r+1} - u_{2n-3} z^{2n-2} -$$

$$- \sum_{\substack{r=1,\\ r \text{ odd}}}^{2n-1} u_r z^{r-1} + \sum_{\substack{r=2,\\ r \text{ even}}}^{2n-4} \varepsilon_{\frac{1}{2}r+1} z^r + u_{2n-3} z^{2n-2} + \varepsilon_n z^{2n-2} +$$

$$+ \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} u_r (z^{r+1} - z^{r-1}) = \left(z - \frac{1}{z}\right) \Theta - u_1 + \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \varepsilon_{\frac{1}{2}r+1} z^r .$$

$$\begin{aligned} \Theta &= \Theta(z,0) \exp\left[\frac{1}{2}\left(z - \frac{1}{z}\right) t\right] + \\ &+ \frac{1}{2} \int_0^t \left[-u_1(s) + \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \varepsilon_{\frac{1}{2}r+1} z^r\right] \exp\left[\frac{1}{2}\left(z - \frac{1}{z}\right)(t-s)\right] ds. \end{aligned}$$

Observe now that

$$\exp\left[\frac{1}{2}\left(z - \frac{1}{z}\right)\tau\right] = \sum_{m=-\infty}^{+\infty} J_m(\tau) z^m \quad \text{for } z \in \mathbb{C}\backslash\{0\},\ \tau \in \mathbb{R} \text{ or } \mathbb{C},$$

$J_{-n}(z) = (-1)^n J_n(z)$ for $n \in \mathbb{Z}$, and $J_{n+1}(\tau) = 2(n/\tau) J_n(\tau) - J_{n-1}(\tau)$ for $n \in \mathbb{Z}$. Hence

$$\sum_{k=0}^{2n-1} u_k(t) z^k = \sum_{k=-\infty}^{+\infty} \left[\sum_{r=0}^{2n-1} J_{k-r}(t) u_r(0) z^k - \right.$$

$$\left. - \frac{1}{2} \int_0^t J_k(t-s) u_1(s) z^k ds + \frac{1}{2} \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \int_0^t J_{k-r}(t-s) \varepsilon_{\frac{1}{2}r+1}(s) z^k ds \right]$$

and, by comparison of the proper coefficients on the both sides, formula (7) follows.

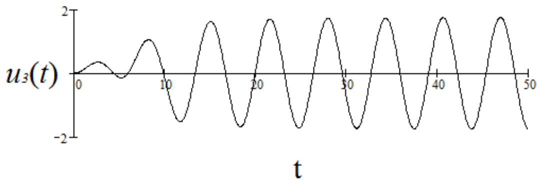

Fig. 1. The relative distance $u_3(t)$ for $n = 4$, and $\varepsilon_1(t) = \varepsilon_4(t) = \cos t$, $\varepsilon_2(t) = \varepsilon_3(t) = \sin 2t$, $u_0(0) = u_7(0) = 5 \cdot 10^{-9}, u_1(0) = u_6(0) = 3 \cdot 10^{-9}$, $u_2(0) = u_5(0) = 2 \cdot 10^{-9}, u_3(0) = u_4(0) = 10^{-9}$.

Physically, u_3 represents the relative distance between the atoms in the third layer; an example is shown in Fig. 1.

3. Extended k **th-Layer Theorem.** With the help of formula (7) we may express, in an analogous way, the other functions u_k in (6). Namely, we have

Theorem 2. *For the sake of simplicity we confine ourselves to the case* (5). *The functions* u_k *in the solution* (6) *of the system of* (3), $r \neq 1$, *and* (4) *can be expressed as*

- *for* $k = 1, 3, ..., 2n-1$

$$u_k(t) = (-1)^{\frac{1}{2}(k+1)} \sum_{\substack{m=1,\\ m \text{ odd}}}^{k} (-1)^{\frac{1}{2}(m+1)} \int_0^t \frac{m-1}{t-s} J_{m-1}(t-s) u_1(s) ds -$$

$$-(-1)^{\frac{1}{2}(k+1)} \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \sum_{\substack{m=1,\\ m \text{ odd}}}^{k} (-1)^{\frac{1}{2}(m+1)} \int_0^t \frac{r+1-m}{t-s} J_{r+1-m}(t-s) \varepsilon_{\frac{1}{2}r+1}(s) ds -$$

$$-2(-1)^{\frac{1}{2}(k+1)} \sum_{r=0}^{2n-1} (-1)^r \sum_{\substack{m=1,\\ m \text{ odd}}}^{k} (-1)^{\frac{1}{2}(m+1)} \frac{r+1-m}{t} J_{r+1-m}(t) u_r(0), \quad (8)$$

- *for* $k = 0, 2, ..., 2n-2$

$$u_k(t) = (-1)^{\frac{1}{2}k} \sum_{\substack{m=0,\\ m \text{ even}}}^{k} (-1)^{\frac{1}{2}m} \int_0^t \frac{m-1}{t-s} J_{m-1}(t-s) u_1(s) ds -$$

$$-(-1)^{\frac{1}{2}k} \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \sum_{\substack{m=0,\\ m \text{ even}}}^{k} (-1)^{\frac{1}{2}m} \int_0^t \frac{r+1-m}{t-s} J_{r+1-m}(t-s) \varepsilon_{\frac{1}{2}r+1}(s) ds -$$

$$-2(-1)^{\frac{1}{2}k} \sum_{r=0}^{2n-1} (-1)^r \sum_{\substack{m=0,\\ m \text{ even}}}^{k} (-1)^{\frac{1}{2}m} \frac{r+1-m}{t} J_{r+1-m}(t) u_r(0) . \quad (9)$$

Proof. By Theorem 1, the general formula for k odd reads:

$$u_k(t) = \sum_{r=0}^{2n-1} (-1)^{r+1} \left[(-1)^{\frac{1}{2}(k+1)} \left(J_{r+1}(t) - J_{r-k}(t) \right) \right] u_r(0) +$$

$$+\frac{1}{2} \int_0^t \left[J_1(t-s) - (-1)^{\frac{1}{2}(k+1)} J_k(t-s) \right] u_3(s) ds -$$

$$-\frac{1}{2} \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \int_0^t \left[(-1)^{\frac{1}{2}(k+1)} \left(J_{r+1}(t-s) - J_{r-k}(t-s) \right) \right] \varepsilon_{\frac{1}{2}r+1}(s) ds$$

and hence (8) follows. In analogy, the general formula for k even reads:

$$u_k(t) = \sum_{r=0}^{2n-1} (-1)^{r} \left[(-1)^{\frac{1}{2}k} J_{r+2}(t) + J_{r-k}(t) \right] u_r(0) -$$

$$-\frac{1}{2} \int_0^t \left[J_2(t-s) - (-1)^{\frac{1}{2}k} J_k(t-s) \right] u_3(s) ds -$$

$$-\frac{1}{2} \sum_{\substack{r=0,\\ r \text{ even}}}^{2n-2} \int_0^t \left[(-1)^{\frac{1}{2}k} J_{r+2}(t-s) - J_{r-k}(t-s) \right] \varepsilon_{\frac{1}{2}r+1}(s) ds$$

and hence (9) follows. Physically, u_k represents the relative distance between the atoms in the k th layer; an example is shown in Fig. 2.

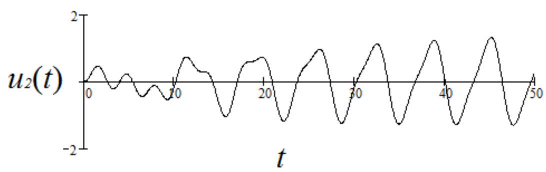

Fig. 2. The relative distance $u_2(t)$ for $n = 4$, and $\varepsilon_1(t) = \varepsilon_4(t) = \cos t$, $\varepsilon_2(t) = \varepsilon_3(t) = \sin 2t$, $u_0(0) = u_7(0) = 5 \cdot 10^{-9}, u_1(0) = u_6(0) = 3 \cdot 10^{-9}$, $u_2(0) = u_5(0) = 2 \cdot 10^{-9}, u_3(0) = u_4(0) = 10^{-9}$.

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