PRAMANA — journal of physics
© Indian Academy of Sciences
Vol. 80, No. 6
June 2013
pp. 1017–1030

Solitary heat waves in nonlinear lattices with squared on-site potential

ROVINITA PERSEUS* and M M LATHA
Women's Christian College, Nagercoil 629 001, India
*Corresponding author. E-mail: rovinita@gmail.com

MS received 6 October 2012; accepted 12 February 2013

Abstract. A model Hamiltonian is proposed for heat conduction in a nonlinear lattice with squared on-site potential using the second quantized operators and averaging the same using a suitable wave function, equations are derived in discrete form for the field amplitude and the properties of heat transfer are examined theoretically. Numerical analysis shows that the propagation of heat is in the form of solitons. Furthermore, a systemized version of tanh method is carried out to extract solutions for the resulting nonlinear equations in the continuum case and the effect of inhomogeneity is studied for different temperatures.

Keywords. Solitons; on-site potential; Schrödinger's equation.

PACS Nos **44.10.+i; 44.90.+c; 44.05.+e; 05.10.−a**

1. Introduction

Currently, there is considerable interest in controlling heat flow in electronic devices, since rapid rise in temperature could wear off the device with time. Scientists have proposed simple linear lattice models and have investigated the heat transfer by attaching thermal sources across the ends of the lattice [1–9]. These simple linear models have been extended to the nonlinear lattice models of one, two and three dimensions to describe the energy transfer more accurately [10–19]. The nonlinearity property is found very useful in controlling heat flow and using this property, thermal rectifiers, diodes and transistors have been designed [20–22]. The thermal transistors consist of three terminals, and by adjusting the temperature of the third terminal, one can amplify current through the other two terminals. This can be used as an efficient heat pump to dissipate heat from a microelectronic or nanoelectronic device where large amount of heat is produced due to the fast operational speed of the device. If the heat is not dissipated immediately, it may wear off the device. By using the nonlinearity property in controlling heat flow a theoretical model of a thermal rectifier has been recently proposed [23–25] in which

DOI: 10.1007/s12043-013-0541-4; ***e*Publication: 25 May 2013**

heat can flow preferentially in one direction. In nonlinear systems, the soliton concept was firmly established as a mode of wave propagation and the conduction of heat in the form of solitons was confirmed by Toda [26]. However, all the studies are based on classical theories. Classical molecular dynamic simulations are restricted to high temperatures [27] though they can incorporate anharmonic interactions to all orders. The mixed classical simulations are valid only at high temperatures or at weak interactions [28,29]. The description of quantum thermal transport across hybrid nanoscale objects were done by Wu and Segal [30] recently in quantum heat transfer studies and they have developed a Born–Oppenheimer type formalism. They have found that the vibrational or electronic energy dynamics could be described in a new way by incorporating quantum effects and nonlinearities. However, the quantum heat conduction in nonlinear lattices based on analytical studies is not fully explored compared to the classical theory and have not been reported in the literature yet. This has prompted us to apply the principles of quantum mechanics to theoretically investigate the dynamics of heat transfer in nonlinear lattices.

The nonlinear lattices play vital roles for constructing electronic devices and optical fibre communication systems. Hence we give special consideration to it. The volumetric rise in temperature must be dissipated very efficiently because the heat formed by Joule effect in these devices will raise the temperature to a very high level which can cause possible failures of the systems. A better understanding of the dynamics of heat conduction may also lead to potentially interesting applications based on the possibility to control the heat flow. As good knowledge of the phenomena governing the heat transfer must be gained in order to achieve this task, we performed thorough investigations on heat conduction in nonlinear lattices. The presence of impurities, defects or imperfections in fact gives rise to inhomogeneities which in turn influence the propagation of heat. Hence both homogeneous and inhomogeneous nonlinear lattices were taken into account for our study.

Our overriding concern is about the role of nonlinearity in the conduction of heat which leads to the emergence of stable localized structures. We have adopted a standard approach using quantum field theory to study the quantum mechanical effects. The main aim of this approach is to follow the method of coherent structures first, i.e. to calculate the Heisenberg equations of motion for the second quantized operators which are required to obey commutation relations. By proposing a model Hamiltonian using the second quantized operators of quantum field theory and after averaging the Hamiltonian using a suitable wave function, we derive the equations for the field amplitude. The resulting nonlinear equation in its natural form is very difficult to solve because of its high nonlinearity and discreteness. Hence we analyse it numerically and in addition we go for the continuum limit. Since the on-site potential is sufficient to ensure the validity of Fourier's law, we analyse the nature of heat conduction in lattices with squared on-site potential. We solve the resulting equations in the continuum limit using perturbation technique and study the effect of inhomogeneity in heat conduction.

This paper is organized as follows. Section 2 deals with the dynamics of heat transfer in the homogeneous nonlinear lattice in the discrete level and §3 deals with the heat conduction in the inhomogeneous one. Section 4 describes the heat transfer in homogeneous and inhomogeneous nonlinear lattices in the continuum level and the conclusion is given in §5.

2. Homogeneous nonlinear lattice

We consider N atoms of identical mass m connected to each other in a homogeneous nonlinear lattice (NL). The Hamiltonian which describes the heat transport is given by [31]

$$H = \sum_{n=1}^{N} \frac{p_n^2}{2m} + U(x_n) + \sum_{n=0}^{N} V(x_{n+1}, x_n)\,, \tag{1}$$

where p_n denotes the momentum operator and x_n is the nth atom's coordinate with lattice constant L. The on-site potential term $U(x_n)$ and the interparticle interaction potential term $V(x_{n+1}, x_n)$ are expressed as

$$U(x_n) = \frac{k'}{2}(x_n)^2\,, \tag{2}$$

$$V(x_{n+1}, x_n) = \frac{k}{2}(x_{n+1} - x_n - L)^2 + \frac{\beta}{4}(x_{n+1} - x_n - L)^4\,, \tag{3}$$

where k' and k are the squared on-site potential and interparticle interaction potential strengths respectively and β is the quantum interparticle interaction potential strength. We now make a transition to a second quantized formalism to bring out the nonlinearity and hence we bozonize the Hamiltonian (1) using the relations

$$p_n = i\sqrt{\frac{m\hbar\omega}{2}}(B_n^{\dagger} - B_n), \tag{4}$$

$$x_n = \rho(B_n + B_n^{\dagger}), \tag{5}$$

where ω is the angular frequency and $\rho = \sqrt{\hbar/2m\omega}$. The bosonic operators B_n and $B_n^{\dagger}$ satisfy the usual commutation relations $[B_m, B_n^{\dagger}] = \delta_{m,n}$, $[B_m, B_n] = [B_m^{\dagger}, B_n^{\dagger}] = 0$. Using eqs (4) and (5), the Hamiltonian (1) can be written as

$$\begin{aligned} H = & \sum_{n=1}^{N} \frac{-\hbar\omega}{4}(B_n^{\dagger 2} - B_n^2) + \frac{k'}{2}\rho^2(B_n + B_n^{\dagger})^2 \\ & + \sum_{n=0}^{N} \frac{k}{2}[\delta(\rho^2\delta - L\tau) + L^2] \\ & + \sum_{n=0}^{N} \frac{\beta}{4}\left[(\rho\delta)^4 - 4L(\rho\delta)^3 + 6(\rho L\delta)^2 - 4L^3\rho\delta + L^4\right], \end{aligned} \tag{6}$$

where $\delta = B_{n+1} + B_{n+1}^{*} - (B_n + B_n^{*})$ and $\tau = \sqrt{2\hbar/m\omega}$. In particular, we are concerned with nonlinear excitations of atoms due to nonlinearity in the system in which a cluster of atoms may undergo a large excursion as compared to the rest of the atoms. Physically, the quantum state of such large-amplitude collective modes may be represented by coherent states. Hence we introduce the coherent state representation [32] of a harmonic oscillator as

$$|u\rangle = \exp\left(-\frac{|B_n|^2}{2}\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle, \tag{7}$$

where α is the eigenvalue corresponding to the eigenvector $|u\rangle$. Using the Glauber formula [33], eq. (7) can be rewritten as

$$|u\rangle = \exp(\alpha B_n^\dagger - \alpha^* B_n)|0\rangle, \tag{8}$$

where $|0\rangle$ is the vacuum state wave function. We now construct the equation of motion for the boson operator using the equations

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\langle B_n\rangle = \langle [B_n, H]\rangle \tag{9}$$

and

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\langle B_n^\dagger\rangle = \langle [B_n^\dagger, H]\rangle. \tag{10}$$

For the bosonic operators, $B_n^\dagger|u\rangle = a_n^*|u\rangle$, $B_n|u\rangle = a_n|u\rangle$ with $\langle u|u\rangle = 1$, where a_n is the coherent amplitude of the operator B_n for the system in the state $|u\rangle$. Now we write down the equation of motion using eqs (6), (9) and (10) as

$$\begin{aligned} i\hbar \frac{\mathrm{d}a_n}{\mathrm{d}t} = & \frac{-\hbar\omega}{2}\left(a_n^* - a_n\right) + k'\rho q + k\rho^2(2q - r - s) + \frac{kL^2}{2} \\ & + \beta\rho^4\left(2q^3 - r^3 - s^3 - 3q^2 r + 3r^2 q + 3s^2 q - 3q^2 s\right) \\ & - 3L\beta\rho^3\left(r^2 - s^2 - 2qr + 2qs\right) \\ & + 3L^2\beta\rho^2(2q - r - s) + \frac{L^4\beta}{4}, \end{aligned} \tag{11}$$

where $q = a_n + a_n^*$, $r = a_{n-1} + a_{n-1}^*$ and $s = a_{n+1} + a_{n+1}^*$ and the numerical study of eq. (11) shows that the heat dissipation in homogeneous nonlinear lattice is in the form of solitons and is shown in figure 1. The two-soliton collision results in the formation of a single wave which ultimately splits up into two and propagates along two opposite directions of the lattice simultaneously resulting in the tremendous enhancement of the amplitude decay rate within a few seconds following the excitation. To some extent, studies based on spatial temperature variation merit more generous description of high solitary peaks in lattices exhibiting high temperature. In a system with higher temperature, the heat transfer is found to be faster than that in a system kept at low temperature. The system parameters are $k = \omega = \beta = 1$ and $m = 28.09$ M/g/mole and the lattice constants are $L = 5.4306$ Å at 320 K and $L = 5.4308$ Å at 310 K.

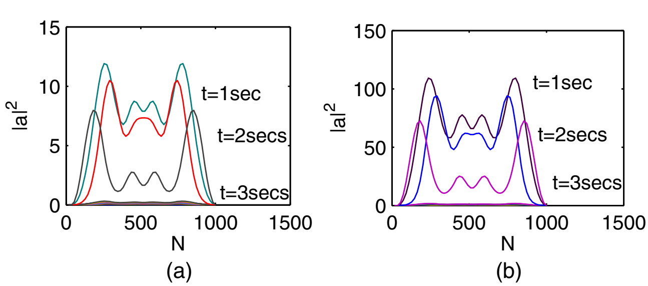

Figure 1. Solitons in a homogeneous NL at (**a**) 310 K and (**b**) 320 K.

3. Inhomogeneous nonlinear lattice

In this section, we study numerically an inhomogeneous nonlinear lattice consisting of N atoms of identical mass m. This set-up is described by the nonlinear lattice Hamiltonian (1) and the potential term $V(x_{n+1}, x_n)$ with inhomogeneities f_n and g_n assumes the following form:

$$V(x_{n+1}, x_n) = \left[\frac{k}{2} f_n \, (x_{n+1} - x_n - L)^2 + \frac{\beta}{4} g_n \, (x_{n+1} - x_n - L)^4\right]. \tag{12}$$

Using the momentum and position operators comprising the annihilation and creation operators, we get

$$\begin{aligned} H &= \sum_{n=1}^{N} \frac{-\hbar\omega}{4}(B_n^\dagger - B_n)^2 + \frac{k'}{2}\rho^2(B_n + B_n^\dagger)^2 \\ &\quad + \sum_{n=0}^{N} \frac{k}{2}\left[\rho^2 f_n \delta^2 - L\tau f_n \delta + L^2\right] \\ &\quad + \sum_{n=0}^{N} \frac{\beta}{4}\left[g_n \, (\rho\delta)^4 - 4L\rho^3 g_n \delta^3 + 6 g_n (L\rho\delta)^2 - 4L^3 \rho g_n \delta + L^4\right]. \end{aligned} \tag{13}$$

The following analysis can be extended by the application of commutations at the expense of heavier calculations

$$\begin{aligned} i\hbar \frac{\mathrm{d}a_n}{\mathrm{d}t} &= \frac{-\hbar\omega}{2}(a_n^* - a_n) + k'\rho(a_n + a_n^*) \\ &\quad + \frac{k}{2}\left[\frac{\hbar}{m\omega}(f_{n-1}z + f_n y) + L\tau(f_n - f_{n-1}) + L^2\right] \\ &\quad + \frac{\beta}{4}\left[\frac{\hbar^2}{m^2\omega^2}(g_{n-1}z^3 + g_n y^3) - 12L\rho^3(g_{n-1}z^2 - g_n y^2)\right. \\ &\quad \left. - 4L^3\rho(g_{n-1} - g_n) + 12L^2\rho^2(g_{n-1}z + g_n y) + L^4\right], \end{aligned} \tag{14}$$

where $y = q - r$ and $z = q - s$. Equation (14) is the discrete equation in which the periodic inhomogeneities are prescribed values as $f_n = g_n = \tanh(n^* h)$ and the system parameters are $k = \omega = \beta = 1$ and $m = 28.09$ M/g/mole and the lattice constants are $L = 5.4341$ Å at 500 K and $L = 5.4431$ Å at 1000 K. Some structural imperfections which modify the character and shape of solitons due to inhomogeneities are inevitable during the fabrication of the lattice. Our further interest with respect to the general understanding of nonlinear phenomena is the behaviour of the system in the neighbourhood of the periodic inhomogeneities which are significant enough to make the nonlinear effects important. At high temperatures, heat energy exchange takes place most efficiently resulting in phase shift with the emission of radiation, due to the inelastic collision of two solitons in the inhomogeneous lattice as shown in figure 2. Solitons remain unaffected by collision except for acquiring a phase shift. Two solitons attract each other when they

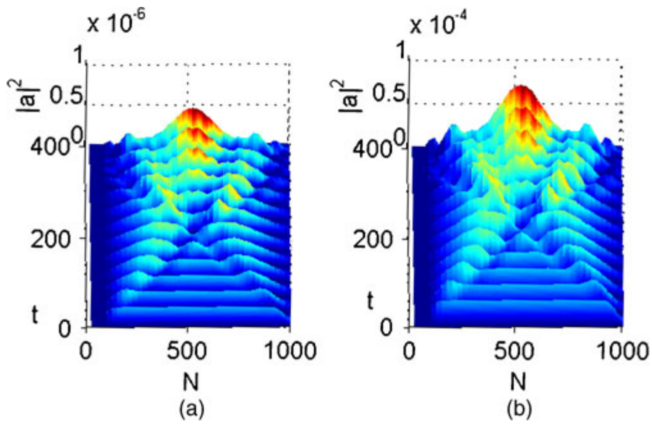

Figure 2. Soliton collision in an inhomogeneous NL at (**a**) 500 K and (**b**) 1000 K.

are in phase, and fuse together when the collision angle is below a certain critical value. Two out-of-phase solitons repel each other and the soliton interaction is accompanied by a strong energy exchange; in the most dramatic case, one of the solitons can even disappear. Even a relatively small perturbation can create an internal mode of the soliton. The soliton-based numerical studies in lattices for low and high thermal conductance reveal the transfer of solitary heat waves in the nonlinear lattice.

4. Continuum level

4.1 *Homogeneous nonlinear lattice*

A systemized version of the tanh method is used to solve the heat wave equations where one seeks solutions in the form of a finite series in tanh and thus obtain exact closed form solutions. The function a_n changes smoothly over one end of the lattice and hence we can replace $a_n(t)$ by $a(x,t)$ and proceed to the continuum limit using the Taylor series expansion

$$a_{n\pm 1} = 1 \pm h a_x + \frac{h^2 a_{xx}}{2!} \pm \frac{h^3 a_{xxx}}{3!} + \frac{h^4 a_{xxxx}}{4!} \pm \cdots, \tag{15}$$

where h is the lattice parameter. Using eq. (15), eq. (14) takes the form

$$\begin{aligned} i\hbar \frac{\mathrm{d}a}{\mathrm{d}t} &= -\frac{\hbar\omega}{2}(a^* - a) + k'\rho w - \frac{4k\pi^2\hbar^3}{m\omega}\left(\frac{1}{2!}w_{xx} + \frac{h^2}{4!}w_{xxxx}\right) \\ &\quad + \frac{kL^2}{2} - \frac{12\hbar^6\beta\pi^4}{m^2\omega^2} w_{xx}(w_x^2 + 2a_x^* a_x) + 6Lh^3\beta\rho^3 (w_x w_{xx}) \\ &\quad - 6L^2h^2\beta\rho\left(\frac{1}{2}w_{xx} + \frac{1}{4!}w_{xxxx}\right) + \frac{L^4\beta}{4}, \end{aligned} \tag{16}$$

where $w = a + a^*$. Using $a = U + iV$, eq. (16) is reduced to the following crucial step and by substituting the imaginary part into the real one we get

$$AU_{tt} + BU - EU_{xx} - FU_{xxxx} + G - HU_{xx} - IU_{xxxx} - JU_x^2 U_{xx} + KU_x U_{xx} + N = 0, \tag{17}$$

where

$$A = \frac{\hbar}{\omega}, \quad B = \frac{k'\hbar}{m\omega}, \quad E = \frac{4k\pi^2\hbar^3}{m\omega}, \quad F = \frac{kh^2\hbar^3\pi^2}{3m\omega},$$
$$G = \frac{kL^2}{2}, \quad H = 6L^2h^2\beta\rho, \quad I = \frac{L^2h^4\beta}{2},$$
$$J = \frac{96\hbar^6\beta\pi^4}{m^2\omega^2}, \quad K = 24L^2h^3\beta\rho^3, \quad N = \frac{L^4\beta}{4}. \tag{18}$$

Equation (17) is a nonintegrable equation which can only be solved using perturbation techniques and for the present study we employ the tanh method which leads to a further systemization of the method and seek solutions in the travelling frame of ref. [34]

$$\xi = \sum_{j=1}^{N}(c_j x_j), \tag{19}$$

where the components c_j of the wave vector x are constants. We seek polynomial solutions expressible in hyperbolic tangent $T = \tanh(\xi)$. Based on the identity $\cosh^2(\xi) - \sinh^2(\xi) = 1$,

$$\tanh'(\xi) = \mathrm{sech}^2(\xi) = 1 - \tanh^2(\xi), \tag{20}$$

$$\tanh''(\xi) = -2\tanh(\xi) + 2\tanh^3(\xi), \qquad \text{etc.} \tag{21}$$

Therefore the first and consequently all higher order derivatives are polynomial in T. Thus, by repeatedly applying the chain rule

$$\frac{\partial \bullet}{\partial x_j} = \frac{\partial \xi}{\partial x_j}\frac{\mathrm{d}T}{\mathrm{d}\xi}\frac{\mathrm{d}\bullet}{\mathrm{d}T} = c_j(1 - T^2)\frac{\mathrm{d}\bullet}{\mathrm{d}T}, \tag{22}$$

eq. (17) is transformed into a coupled system of nonlinear ODEs

$$\Gamma(T, U(T), U'(T), \ldots) = 0, \tag{23}$$

where $U_n(T)$ corresponds to $a_n(x)$. Using this technique, eq. (17) is reduced to a nonlinear ODE as follows:

$$Ac_2^2[U'\phi_2 + U''\phi_1] + BU - Ec_1^2[U'\phi_2 + U''\phi_1] - Fc_1^4[U'\phi_3 + U''\phi_4 + U'''\phi_5 + U''''\phi_6] - Hc_1^2[U'\phi_2 + U''\phi_1] - Ic_1^4[U'\phi_3 + U''\phi_4 + U'''\phi_5 + U''''\phi_6] - Jc_1^4[U'U'^2\phi_7 + U''U'^2\phi_6] + Kc_1^3[U'U''\phi_8 + U'^2(\phi_9)] + N + G = 0, \tag{24}$$

where

$$\phi_1 = 1-2T^2+T^4, \quad \phi_2 = -2T+2T^3, \quad \phi_3 = 16T-40T^3+24T^5,$$

$$\phi_4 = -8+52T^2-80T^4+36T^6, \quad \phi_5 = -12T+36T^3-36T^5+12T^7,$$

$$\phi_6 = 1-4T^2+6T^4-4T^6+T^8, \quad \phi_7 = -2T+6T^3-6T^5+2T^7,$$

$$\phi_8 = 1-3T^2+3T^4-T^6, \quad \phi_9 = -2T+4T^3-2T^5. \tag{25}$$

The tanh method admits the use of the finite expansion

$$U(T) = \sum_{j=0}^{M}(a_j T^j). \tag{26}$$

Balancing the linear and nonlinear terms gives $M = 1$. Equating the coefficients of the powers of T, we get

$$G+N+Ba_0 = 0, \tag{27}$$

$$Ba_1 - 2c_2^2 a_1 A + 2Ec_1^2 a_1 - 16Fc_1^4 a_1 + 2Hc_1^2 a_1 - 16Ic_1^4 a_1 + 2Jc_1^4 a_1^3 - 2Kc_1^3 a_1^2 = 0, \tag{28}$$

$$2Ac_2^2 a_1 - 2Ec_1^2 a_1 + 40Fc_1^4 a_1 - 2Hc_1^2 a_1 + 40Ic_1^4 a_1 - 6Jc_1^4 a_1^3 + 4Kc_1^3 a_1^2 = 0, \tag{29}$$

$$-24Fc_1^4 a_1 - 24Ic_1^4 a_1 + 6Jc_1^4 a_1^3 - 2Kc_1^3 a_1^2 = 0, \tag{30}$$

$$-2Jc_1^4 a_1^3 = 0. \tag{31}$$

Assuming $J = 0$ and $a_1 \neq 0$,

$$a_1 = \frac{B - 2Ac_2^2 + 2Ec_1^2 - 16Fc_1^4 + 2Hc_1^2 - 16Ic_1^4}{2Kc_1^3}, \tag{32}$$

$$a_0 = \frac{-G-N}{B}. \tag{33}$$

Customized conditions are designed as follows to solve the above equations:

$$E = \frac{2Ka_1c_1^3 + Ac_3^2 + 20Fc_1^4 - Hc_1^2 + 20Ic_1^4}{c_1^2}, \tag{34}$$

and

$$K = \frac{-12Fc_1 - 12Ic_1}{a_1}. \tag{35}$$

By solving the equations we obtain the explicit solution as

$$U = \frac{-G-N}{B} + \left(\frac{B - 2Ac_2^2 + 2Ec_1^2 - 16Fc_1^4 + 2Hc_1^2 - 16Ic_1^4}{2Kc_1^3}\right) \times \tanh(c_1 x + c_2 t). \tag{36}$$

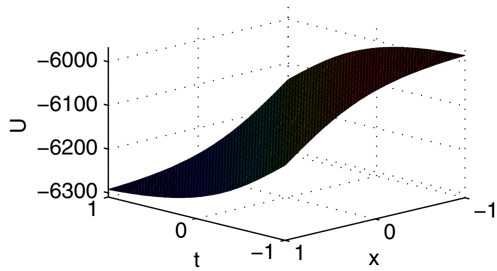

Figure 3. Soliton in a homogeneous nonlinear lattice at 500 K.

Equation (36) gives the travelling wave solution and it admits kink-like propagation which is a form of a soliton. The propagation of a soliton in the homogeneous nonlinear lattice at 500 K for the lattice parameters $c_1 = c_2 = 1$ is shown in figure 3.

4.2 *Inhomogeneous nonlinear lattice*

The powerful tanh method provides an effective way to construct the solitary wave solutions. The following equation can thus be obtained by the pure application of continuous approximation technique.

$$
\begin{aligned}
i\hbar \frac{\mathrm{d}a}{\mathrm{d}t} = \; & \alpha_1(a^* - a) + k'\rho(a + a^*) \\
& + \alpha_2\Big(-2fe^2w_{xx} - 2f_xe^2w_x + f_xe^3w_{xx} + e^3f_{xx}w_x - \frac{1}{2}f_{xx}e^4w_{xx} \\
& \quad - \frac{1}{3}f_{xxx}e^4w_x - \frac{1}{3}f_xe^4w_{xxx} - \frac{1}{6}fe^4w_{xxxx}\Big) \\
& + \alpha_3\left(f_xe - \frac{1}{2}f_{xx}e^2 + \frac{1}{6}f_{xxx}e^3 - \frac{1}{24}f_{xxxx}e^4\right) + \frac{kL^2}{2} \\
& + \alpha_4\left(-3a_x^2ge^4w_{xx} - g_xe^4w_x^3 - 6a_xge^4a_x^*w_{xx} - 3ge^4a_x^{*2}w_{xx}\right) \\
& + \alpha_5\Big(-g_xe^3w_x^2 - 2a_{xx}^*ge^3w_x - 2a_{xx}ge^3w_x + a_{xx}g_xe^4w_x \\
& \quad + \frac{1}{2}g_{xx}e^4w_x^2 + g_xe^4a_{xx}^*w_x\Big) \\
& + \alpha_6\left(-g_xe + \frac{1}{2}g_{xx}e^2 - \frac{1}{6}g_{xxx}e^3 + \frac{1}{24}g_{xxxx}e^4\right) \\
& + \alpha_7\Big[\left(4wg - 2wg_xe + wg_{xx}e^2 - \frac{1}{3}g_{xxx}e^3w + \frac{1}{12}g_{xxxx}e^4w\right) \\
& \quad - 2\Big(2gw - g_xew + ge^2w_{xx} + \frac{1}{2}wg_{xx}e^2 + g_xe^2w_x
\end{aligned}
$$

$$-\frac{1}{2}g_x e^3 w_{xx} - \frac{1}{2}g_{xx} e^3 w_x - \frac{1}{6} w g_{xxx} e^3 + \frac{1}{12} g e^4 w_{xxxx}$$
$$+\frac{1}{6} g_x e^4 w_{xxx} + \frac{1}{4} g_{xx} e^4 w_{xx} + \frac{1}{6} g_{xxx} e^4 w_x$$
$$+\frac{1}{24} g_{xxxx} e^4 w_x \Bigg) \Bigg] + \frac{L^4\beta}{4}, \tag{37}$$

where

$$\alpha_1 = \frac{-\hbar\omega}{2}, \qquad \alpha_2 = \frac{k\rho^2}{2}, \qquad \alpha_3 = \frac{kL}{2}\tau, \qquad \alpha_4 = \beta\rho^4,$$
$$\alpha_5 = -3L\beta\rho^3, \qquad \alpha_6 = -L^3\beta\rho, \qquad \alpha_7 = \frac{3L^2\beta}{2}\rho, \tag{38}$$

and e is the lattice parameter. Equation (37) can be consequently reduced to the following form by using $a = U + iV$ and substituting the imaginary part into the real part, we get

$$D_1 U_{tt} + D_2 U + s_1 U_x + s_2 U_{xx} - s_3 U_{xxx} - s_4 U_{xxxx} + D_{11} U_x U_{xx}$$
$$- D_{12} U_{xxx} U_x - D_9 U_x^2 U_{xx} + D_{10} U_x^2 - D_8 U_x^3 + D_7 + D_{17} = 0, \tag{39}$$

where

$$D_1 = \frac{\hbar}{\omega}, \qquad D_2 = \frac{k'\hbar}{m\omega}, \qquad D_3 = \frac{ke^4 f_x \hbar}{6m\omega},$$
$$D_4 = -\frac{ke^2 f_x \hbar}{m\omega} + \frac{ke^3 f_{xx}\hbar}{2m\omega} - \frac{ke^4 f_{xxx}\hbar}{6m\omega},$$
$$D_5 = -\frac{ke^2 f\hbar}{m\omega} + \frac{ke^3 f_x\hbar}{2m\omega} - \frac{ke^4 f_{xx}\hbar}{4m\omega}, \qquad D_6 = \frac{ke^4 f\hbar}{12m\omega},$$
$$D_7 = \frac{kLef_x\hbar}{4m\omega}\tau - \frac{kLe^2 f_{xx}\hbar}{8m\omega}\tau + \frac{kLe^3 f_{xxx}\hbar}{24m\omega}\tau$$
$$- \frac{kLe^4 f_{xxxx}\hbar}{96m\omega}\tau + \frac{kL^3\hbar}{4m\omega}\tau,$$
$$D_8 = \frac{2e^4 g_x \beta\hbar^2}{m^2\omega^2}, \qquad D_9 = \frac{6e^4 g\beta\hbar^2}{m^2\omega^2},$$
$$D_{10} = 12Le^3 g_x\beta\rho^3 - 6e^4 L g_{xx}\beta\rho^3, \qquad D_{11} = 24Le^3 g\beta\rho^3,$$
$$D_{12} = 12Le^4 g_x\beta\rho^3, \qquad D_{13} = L^2 e^4 g_x \beta\rho,$$
$$D_{14} = -6e^2 L^2 g_x\beta\rho + 3e^3 L^2 g_{xx}\beta\rho - e^4 L^2 g_{xxx}\beta\rho,$$
$$D_{15} = -6L^2 e^2 g\beta\rho + 3L^2 e^3 g_x\beta\rho - \frac{3L^2 e^4 g_{xx}\beta}{2}\rho,$$
$$D_{16} = \frac{L^2 e^4 g\beta}{2}\rho,$$

$$D_{17} = L^3 e g_x \beta\rho - \frac{L^3 e^2 g_{xx}\beta}{2}\rho + \frac{L^3 e^3 g_{xxx}\beta}{6}\rho$$
$$- \frac{L^3 e^4 g_{xxxx}\beta}{24}\rho + \frac{L^4\beta}{4}.$$
$$s_1 = D_4 + D_{14}, \qquad s_2 = D_5 + D_{15}, \qquad s_3 = D_3 + D_{13},$$
$$s_4 = D_6 + D_{16}. \tag{40}$$

Transformation of eq. (39) into a nonlinear ODE can be done by the repeated application of chain rule.

$$D_1 c_2^2[U'\phi_2 + U''\phi_1] + D_2 - D_3 c_1^3[U'\phi_{10} + U''\phi_{11} + U'''\phi_8]$$
$$+ D_4 c_1 U'\phi_{12} + D_5 c_1^2[U'\phi_2 + U''\phi_1]$$
$$- D_6 c_1^4[U'\phi_3 + U''\phi_4 + U'''\phi_5 + U''''\phi_6] - D_8 c_1^3[U'^3\phi_8]$$
$$- D_9 c_1^4[U'^2 U'\phi_7 + U'^2 U''\phi_6] + D_{10} c_1^2 U'^2\phi_1 + D_{11} c_1^3[U'U''\phi_8 + U'^2\phi_9]$$
$$- D_{12} c_1^4[U''U'(-6T + 18T^3 - 18T^5 + 6T^7) + U'U'''\phi_6$$
$$+U'^2(-2 + 10T^2 - 14T^4 + 6T^6)]$$
$$- D_{13} c_1^3[U'\phi_{10} + U''\phi_{11} + U'''\phi_8] + D_{14} c_1 U'\phi_{12}$$
$$+ D_{15} c_1^2[U'\phi_2 + U''\phi_1] - D_{16} c_1^4[U'\phi_3 + U''\phi_4 + U'''\phi_5 + U''''\phi_6]$$
$$+ D_7 + D_{17} = 0, \tag{41}$$

where

$$\phi_{10} = -2 + 8T^2 - 6T^4, \qquad \phi_{11} = -6T + 12T^3 - 6T^5,$$
$$\phi_{12} = 1 - T^2. \tag{42}$$

Balancing the highest order linear and nonlinear terms leads to $M = 1$ and we have

$$D_7 + D_{17} - D_8 c_1^3 a_1^3 + 2D_{12} c_1^4 a_1^2 + D_{10} c_1^2 a_1^2 + D_4 c_1 a_1 + D_{14} c_1 a_1$$
$$+ 2D_3 c_1^3 a_1 + 2D_{13} c_1^3 a_1 + D_2 a_0 = 0, \tag{43}$$
$$- 16D_6 c_1^4 a_1 - 2D_5 c_1^2 a_1 - 16D_{16} c_1^4 a_1 - 2D_{15} c_1^2 a_1$$
$$+ 2D_9 c_1^4 a_1^3 - 2D_{11} c_1^3 a_1^2 - 2D_1 c_2^2 a_1 + D_2 a_1 = 0, \tag{44}$$
$$- D_4 c_1 a_1 - D_{14} c_1 a_1 - 8D_3 c_1^3 a_1 - 8D_{13} c_1^3 a_1$$
$$+ 3D_8 c_1^3 a_1^3 - 10D_{12} c_1^4 a_1^2 - 2D_{10} c_1^2 a_1^2 = 0, \tag{45}$$
$$2D_1 c_2^2 a_1 + 40D_6 c_1^4 a_1 + 2D_5 c_1^2 a_1 + 40D_{16} c_1^4 a_1$$
$$+ 2D_{15} c_1^2 a_1 - 6D_9 c_1^4 a_1^3 + 4D_{11} c_1^3 a_1^2 = 0, \tag{46}$$
$$6D_3 c_1^3 a_1 + 6D_{13} c_1^3 a_1 - 3D_8 c_1^3 a_1^3 + 14D_{12} c_1^4 a_1^2 + D_{10} c_1^2 a_1^2 = 0, \tag{47}$$

$$-24D_6c_1^4a_1 - 24D_{16}c_1^4a_1 + 6D_9c_1^4a_1^3 - 2D_{11}c_1^3a_1^2 = 0, \tag{48}$$

$$D_8c_1^3a_1^3 - 6D_{12}c_1^4a_1^2 = 0, \tag{49}$$

$$-2D_9c_1^4a_1^3 = 0. \tag{50}$$

Assuming $D_9 = 0$ and $a_1 \neq 0$ we get

$$a_0 = -D_7 - D_{17} + \frac{6c_1D_{12}}{D_8}\left[\frac{36c_1^5D_{12}^2}{D_8} - \frac{72c_1^6D_{12}^3}{D_8^2} - \frac{6c_1^3D_{10}D_{12}}{D_8} - c_1D_4 - c_1D_{14} - 2c_1^3D_3 - 2c_1^3D_{13}\right], \tag{51}$$

$$a_1 = \frac{6D_{12}c_1}{D_8}. \tag{52}$$

Adhering to the conditions

$$D_5 = \frac{D_2 - 16D_6c_1^4 - 16D_{16}c_1^4 - 2D_{15}c_1^2 - 2D_{11}c_1^3a_1 - 2D_1c_2^2}{2c_1^2}, \tag{53}$$

$$D_4 = -D_{14} - 8D_3c_1^2 - 8D_{13}c_1^2 + 3D_8c_1^2a_1^2 - 10D_{12}c_1^3a_1 - 2D_{10}c_1a_1, \tag{54}$$

$$D_1 = \frac{-40D_6c_1^4 - 2D_5c_1^2 - 40D_{16}c_1^4 - 2D_{15}c_1^2 - 4D_{11}c_1^3a_1}{2c_2^2}, \tag{55}$$

$$D_3 = \frac{-6D_{13}c_1 + 3D_8c_1a_1^2 - 14D_{12}c_1^2a_1 - D_{10}a_1}{6c_1}, \tag{56}$$

$$D_6 = \frac{-24D_{16}c_1 - 2D_{11}a_1}{24c_1}, \tag{57}$$

the following solution is obtained by solving the equations from (43) to (50)

$$U(\xi) = -D_7 - D_{17} + \frac{6c_1D_{12}}{D_8}\left[\left(\frac{36c_1^5D_{12}^2}{D_8}\right) - \left(\frac{72c_1^6D_{12}^3}{D_8^2}\right) - \left(\frac{6c_1^3D_{10}D_{12}}{D_8}\right) - c_1D_4 - c_1D_{14} - 2c_1^3D_3 - 2c_1^3D_{13}\right] + \frac{6D_{12}c_1}{D_8} \times \tanh(c_1x + c_2t). \tag{58}$$

The propagation of the solitary pulses at 500 K in the inhomogeneous nonlinear lattice with periodic inhomogeneities ($f_n = g_n = \sin(n)$) is shown in figure 4. Addition of impurities in the lattice structure alters the available quantum states leading to the appearance of new energy levels in the band structure. This produces significant changes in their properties and it is found that as the critical inhomogeneous region is approached, the soliton looses its identity and takes the form of a dispersive wave ultimately resulting in a steady state while the temperature reaches its threshold value.

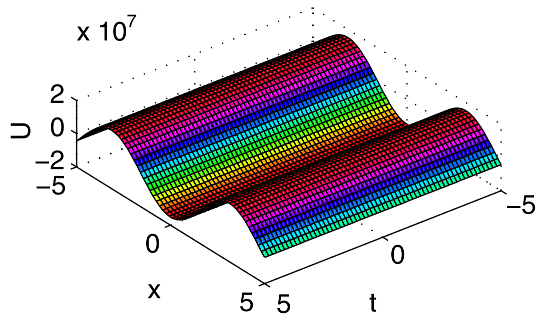

Figure 4. Soliton in an inhomogeneous nonlinear lattice at 500 K.

5. Conclusion

To conclude, we briefly specify the main results of this paper. As far as theoretical work on quantum heat conduction is concerned, the guiding criterion of mathematical simplicity leads naturally to consider homogeneous and inhomogeneous lattices of point-like atoms interacting with their neighbours through nonlinear forces due to rise in temperature. By considering a model Hamiltonian using the second quantized operators of quantum field theory, we derived the equations for the field amplitude and after averaging the Hamiltonian using a suitable wave function, we analysed it numerically and analytically. The numerical results explicitly gave rise to the two-soliton interaction and provided comprehensive information on the exchange interactions. It is found that a quick heat transition takes place in systems with higher temperature. Particular emphasis has been put on the inhomogeneities f_n and g_n in nonlinear lattices which turn out to be a crucial support in enhancing the temperature to reach its threshold value and the analysis on continuum level shows that a steady-state level is reached in the presence of inhomogeneities. Peculiar variations in solitons have been depicted in graphs and the results have been generalized.

Acknowledgement

The work of M M Latha forms part of a major research project sponsored by University Grants Commission (UGC) (F. No. 38-265/2009(SR)), India.

References

[1] H Nakazawa, *Prog. Theor. Phys.* **39**, 236 (1968)
[2] R J Rubin and W L Greer, *J. Math. Phys.* **12**, 1686 (1971)
[3] U Zurcher and P Talkner, *Phys. Rev. A* **42**, 3278 (1990)
[4] W M Visscher and M Rich, *Phys. Rev. A* **12**, 675 (1975)
[5] F Bonetto, J L Lebowitz and J Lukkarinen, *J. Stat. Phys.* **116**, 783 (2004)
[6] D Roy, *Phys. Rev. Lett. E* **77**, 062102 (2008)
[7] T Mai and O Narayan, *Phys. Rev. Lett. E* **73**, 061202 (2006)
[8] S Lepri, R Livi and A Politi, *Europhys. Lett.* **43**, 271 (1998)
[9] L Delfini, *Phys. Rev. Lett. E* **73**, 060201 (2006)

[10] A Dhar, *Phys. Rev. Lett.* **87**, 069401 (2001)
[11] B Li, H Zhao and B Hu, *Phys. Rev. Lett.* **87**, 069402 (2001)
[12] S John, H Sompolinsky and M J Stephen, *Phys. Rev. Lett. B* **27**, 5592 (1983)
[13] Lei Yang, *Phys. Rev. Lett.* **88**, 094301 (2002)
[14] B Hu, Bai-Qi Jin, L Wang and H Yang, *Phys. Rev. Lett.* **90**, 119401 (2003)
[15] L W Lee and A Dhar, *Phys. Rev. Lett.* **95**, 094302 (2005)
[16] S Lepri, R Livi and A Politi, *Phys. Rev. Lett.* **78**, 1896 (2003)
[17] H Zhao, L Yi, F Liu and B Xu, *Eur. Phys. J. B* **54**, 185 (2006)
[18] D N Payton, M Rich and W M Visscher, *Phys. Rev. Lett.* **160**, 706 (1967)
[19] A Lippi and R Livi, *J. Stat. Phys.* **100**, 1147 (2000)
[20] M Buttiker, *Phys. Rev. Lett. B* **33**, 3020 (1986)
[21] B Li, L Wang and G Casati, *Appl. Phys. Lett.* **88**, 143501 (2006)
[22] B Li, L Wang and G Casati, *Phys. Rev. Lett.* **93**, 184301 (2004)
[23] G Casati, C Mejia-Monasterio and T Prosen, *Phys. Rev. Lett.* **98**, 104302 (2007)
[24] D Segal and A Nitzan, *Phys. Rev. Lett.* **94**, 034301 (2005)
[25] M Terraneo, M Peyrard and G Casati, *Phys. Rev. Lett.* **88**, 094302 (2002)
[26] M Toda, *Phys. Scr.* **20**, 424 (1979)
[27] A Dhar, *Adv. Phys.* **57**, 457 (2008)
[28] J S Wang, *Phys. Rev. Lett.* **99**, 160601 (2007)
[29] G Stock, *Phys. Rev. Lett.* **102**, 118301 (2009)
[30] L A Wu and D Segal, *Phys. Rev. E* **83**, 051114 (2011)
[31] N Li, F Zhan, P Hanggi and B Li, *Phys. Rev. E* **80**, 011125 (2009)
[32] J M Radcliffe, *J. Phys. A: Gen. Phys.* **4**, 313 (1971)
[33] R J Glauber, *Phys. Rev.* **131**, 2766 (1963)
[34] D Baldwin, Ü Göktaş and W Hereman, *Comput. Phys. Commun.* **162**, 203 (2004)