Quantum corrections for a system of interacting phonons and the modified Korteweg-de Vries equation

1979 J. Phys. A: Math. Gen. 12 911

(http://iopscience.iop.org/0305-4470/12/6/022)

J. Phys. A: Math. Gen., Vol. 12, No. 6, 1979. Printed in Great Britain

Quantum corrections for a system of interacting phonons and the modified Korteweg–de Vries equation

K Ahmed and G Murtaza
Department of Physics, Quaid-i-Azam University, Islamabad, Pakistan

Received 14 April 1978, in final form 11 September 1978

Abstract. A one-dimensional anharmonic lattice with four phonon interaction is studied. The quantum corrections to the nonlinear equation of motion are calculated and a single soliton-like solution of this equation is obtained in the coherent state representation of phonons.

1. Introduction

Recent interest in the non-linear (anharmonic) lattice system began with the early numerical study of Fermi, Pasta and Ulam (1965), (hereafter denoted by FPU) on the problem of the normal-mode energy behaviour of a system of particles connected by a set of non-linear springs arranged as an approximation to one-dimensional anharmonic coupled oscillators in a lattice. An explanation of the 'energy recurrence' phenomenon observed by FPU and also the absence of equipartition of normal mode energies was later given by Zabusky (1967), on the basis of his continuum model. Toda (1975) has also given a similar explanation using his exponential lattice. Zabusky, however, emphasised the classical wave-like picture, deriving the Korteweg–de Vries (KDV) equation for this nonlinear system and its finite amplitude soliton solution. He has further stressed that the quantum approach based on phonons for this problem is not a suitable way to describe the 'recurrence' phenomenon. More recently, Ichikawa, Yajima and Takano (1976), (hereafter denoted by IYT) in an interesting work have established a correspondence between the non-linear wave phenomenon and the quantum approach based on the phonon description for such a lattice system. Assuming an interaction containing the lowest degree of non-linearity, that is, three, for a one-dimensional lattice, IYT have explicitly derived the KDV equation on the basis of a coherent state representation for the interacting phonons. They further showed explicitly that a soliton can be given a quantum mechanical interpretation as a coherent state of excited phonons in the system. In the present paper we extend their work to the case of fourth degree of anharmonicity. This case is of interest because of its field theoretical importance and its analogy with the self-interacting scalar $\lambda\phi^4$-field theory. As in the $\lambda\phi^4$-theory, one expects here quantum corrections that would modify the frequency $\omega(k)$ of the free oscillator, or, in the language of field theory, 'renormalise' the corresponding phonon energy $\hbar\omega(k)$. Without resort to explicit perturbation

† Presently on leave to the Department of Physics, Faculty of Science, University of Garyounis, Benghazi, Libya.

theory or to Feynman diagrams, we propose to evaluate these effects by introducing the normally ordered Hamiltonian into the framework laid down by IYT. The introduction of the interaction through the time ordering, therefore, generates the required quantum corrections. The resulting equation of motion in the low wave number approximation is still the KDV type. We again obtain a soliton solution of this equation which now depends upon the quantum correction factor. It is also argued that the quantum corrections vanish in the case of non-linearity $n = 3$ to give the same result as that of IYT.

The plan of the paper is as follows: The remaining section reviews the notation of IYT, also to be used here. In § 2, we evaluate the quantum fluctuation contribution to the equation of motion. Next we make a long wavelength approximation of this equation, finally solving it. In § 3 the conclusion and remarks are provided.

We write the Hamiltonian for our anharmonic lattice as

$$H = H_0 + H',$$

where

$$H_0 = \sum_{r=1}^{N} \tfrac{1}{2}[\mu \dot{y}_r^2 + \kappa (y_{r+1} - y_r)^2] \qquad H' = \sum_{r=1}^{N} \tfrac{1}{4}\kappa g_4 (y_{r+1} - y_r)^4 \tag{1.1}$$

and g_4 is the non-linear coupling of fourth degree in our case. The normal mode expansions for atomic displacements are

$$y_r = N^{-1/2} \sum_k (h/2\mu\omega(k))^{1/2} (a^{\dagger}_{-k} + a_k) \exp(\mathrm{i}kx_r) \tag{1.2}$$

where $x_r = rl$ is the position of the rth atom in terms of the lattice spacing constant l. Thus substituting (1.2) into (1.1), we obtain

$$\begin{aligned} H_0 &= \sum_k \hbar\omega(k)(a^{\dagger}_k a_k + \tfrac{1}{2}) \\ H' &= \sum_{k_1,\ldots,k_4} \Delta(k_1 + \ldots + k_4)\phi(k_1, \ldots, k_4)(a^{\dagger}_{-k_1} + a_{k_1}) \ldots (a^{\dagger}_{-k_4} + a_{k_4}) \end{aligned} \tag{1.3}$$

where

$$\begin{aligned} &\Delta(k) = N^{-1} \sum_{r=1}^{N} \exp(\mathrm{i}rlk), \qquad \omega^2(k) = 4\kappa/\mu \sin^2(\tfrac{1}{2}lk), \qquad \omega(-k) = \omega(k) \\ &\phi(k_1, \ldots, k_4) = (\tfrac{1}{4}\kappa g_4)(\hbar/2\mu)^2[(2i)^2/N^{1/2}]^2 \\ &\qquad \times \exp[-\tfrac{1}{2}\mathrm{i}l(k_1 + \ldots + k_4)][\omega(k_1), \ldots, (k_4)]^{-1/2} \sin \tfrac{1}{2}lk_1 \ldots \sin \tfrac{1}{2}lk_4. \end{aligned} \tag{1.4}$$

Lastly, to complete quantisation the quantum relations are given as:

$$[a_k, a^{\dagger}_{k'}] = \Delta(k - k') \qquad [a_k, a_{k'}] = 0 \qquad [a^{\dagger}_k, a^{\dagger}_{k'}] = 0. \tag{1.5}$$

The Glauber (1963) coherent states of phonons $|\alpha_k\rangle$ used as the basic representation by both IYT and ourselves are defined as

$$a_k|\alpha_k\rangle = \alpha_k|\alpha_k\rangle, \qquad |\alpha_k\rangle = \exp(-|\alpha_k|^2) \sum_{n_k=0}^{\infty} (\alpha_k)^{n_k}/(n_k!)^{1/2}|n_k\rangle. \tag{1.6}$$

The average occupation number of phonons n_k is therefore given by the Poisson distribution with mean value of $\langle n_k\rangle = |\alpha_k|^2$. The expectation value of the displacement operator y_r in the coherent state representation is then given by

$$\langle\alpha_k|y_r|\alpha_k\rangle = N^{1/2}\sum_k y(k)\exp(\mathrm{i}kx) \qquad (1.7)$$

using equations (1.2) and (1.6), where the 'amplitude'

$$y(k) = (\hbar/2\mu\omega(k))^{1/2}(\alpha^*_{-k}+\alpha_k).$$

2. Quantum correction contribution to equation of motion

2.1. *Exact derivation*

In order to calculate these effects let us consider the commutator of the operator a_q with the normally ordered interacting part of the Hamiltonian, H':†

$$[a_q, :H':] = 4\sum_{k_1,\ldots,k_4}\phi(k_1,\ldots,k_4)\,\Delta(k_1+\ldots+k_4)\,\Delta(q+k_1)(a^\dagger_{-k_2}+a_{k_2})$$
$$\times(a^\dagger_{-k_3}+a_{k_3})(a^\dagger_{-k_4}+a_{k_4}) + 24\sum_k\phi(-q,k,-k,q)(a^\dagger_{-q}+a_q). \qquad (2.1)$$

Note that the second term in equation (2.1) comes from all possible single contractions. Next the expectation value of equation (2.1) in the coherent state (1.6) describes the equation of motion for the eigenvalue α_k.‡

$$\mathrm{i}h\frac{\partial}{\partial t}\alpha_k = \langle\alpha|[a_k, :H:]|\alpha\rangle$$
$$= \hbar\omega(k)\alpha_k + 4\sum_{k_1,\ldots,k_4}\phi(k_1,\ldots,k_4)\,\Delta(k_1+\ldots+k_4)$$
$$\times\Delta(k+k_2)(\alpha^*_{-k_2}+\alpha_{k_2})(\alpha^*_{-k_3}+\alpha_{k_3})(\alpha^*_{-k_4}+\alpha_{k_4})$$
$$+24(\alpha^*_{-k}+\alpha_k)\sum_{k'}\phi(-k,k',-k',k). \qquad (2.2)$$

Similarly

$$\mathrm{i}h\frac{\partial}{\partial t}\alpha^*_{-k}(t) = -\hbar\omega(k)\alpha^*_{-k} - 4\sum_{k_1,\ldots,k_4}\phi(k_1,\ldots,k_4)\,\Delta(k_1+\ldots+k_4)$$
$$\times\Delta(k+k_1)(\alpha^*_{-k_2}+\alpha_{k_2})(\alpha^*_{-k_3}+\alpha_{k_3})(\alpha^*_{-k_4}+\alpha_{k_4})$$
$$-24(\alpha^*_{-k}+\alpha_k)\sum_{k'}\phi(-k,k',-k',k). \qquad (2.3)$$

† Of course, the normal ordering prescription is more complete field theoretically as it also takes loop divergences into account (see Rajaraman 1975). However, this prescription does not lead to any new result in the case of non-linearity $n = 3$. See the next footnote in this context. Note that the corresponding equation to equation (2.1) in the case of IYT after using normal ordering would not yield any terms additional to those already given there, as contractions in their case give

$$\sum_{k_1,k_2,k_3}\phi(k_1,k_2,k_3)\,\Delta(k_1,k_2,k_3)\,\Delta(k_1+k_2)\,\Delta(k+k_3),$$

which vanishes identically, because of the property of the coupling coefficient

$$(\phi(k_1,k_2,k_3))^2 \propto \sin(\tfrac{1}{2}lk_1)\sin(\tfrac{1}{2}lk_2)\sin(\tfrac{1}{2}lk_3).$$

‡ With IYT, we have neglected the contribution of Umklapp processes in our calculation.

Using equations (1.2′), (2.1) and (2.2), the equation of motion for the kth mode amplitude $y(k)$ after some straightforward calculation becomes:

$$\ddot{y}(k,t) = -\Big(\omega^2(k) + 48(\omega(k)/\hbar)\sum_{k'}\phi(-k,k',-k',k)\Big)y(k,t)$$
$$-8(2\mu/\hbar)^{3/2}(\omega(k)/2\mu\hbar)^{1/2}\sum_{k_1,\ldots,k_4}\phi(k_1,\ldots,k_4)\,\Delta(k_1+\ldots+k_4)$$
$$\times\Delta(k+k_1)(\omega(k_2)\omega(k_3)\omega(k_4))^{1/2}y(k_2,t)y(k_3,t)y(k_4,t) \qquad (2.4)$$

where the second term in brackets containing the sum over k is the required contribution from quantum corrections.

To calculate this quantum correction effect explicitly, we first evaluate the expression for ϕ from (1.4) as

$$\phi(-k,k',-k',k) = C_N\hbar^2\omega(k)\omega(k'),$$

where

$$C_N = N^{-1}(g_4/16\kappa).$$

The equation of motion (2.4) then becomes†

$$\ddot{y}(k,t) = -\omega^2(k)\Big(1+48C_N\,.\,\hbar\sum_{k'}\omega(k')\Big)y(k,t) - 8(2\mu/\hbar)^{3/2}(\omega(k)/2\mu\hbar)^{1/2}$$
$$\times\sum_{k_1,\ldots,k_4}\phi(k_1,\ldots,k_4)\,\Delta(k_1+\ldots+k_4)\,\Delta(k+k_1)$$
$$\times(\omega(k_2)\omega(k_3)\omega(k_4))^{1/2}y(k_2,t)y(k_3,t)y(k_4,t). \qquad (2.5)$$

2.2. Long wavelength approximation

At this stage we introduce the approximation of neglect of large wave number phonons to solve the exact equation (2.5). But before this we notice that the frequency of the free oscillator has now been modified in equation (2.5) due to the quantum corrections according to

$$\omega^2(k) \to \Big(1+48C_N\hbar\sum_{k'}\omega(k')\Big)\omega^2(k) = f^2\omega^2(k) \equiv \omega'^2(k),$$

where

$$f^2 = 1 + 48C_N\hbar\sum_{k'}\omega(k') \qquad (2.5')$$

is the frequency correction factor with

$$\sum_{k'}\omega(k') = (4\kappa/\mu)\sum_{k'}\sin(\tfrac{1}{2}lk'), \qquad \text{(for positive values of } k'\text{)}$$

† It is interesting to observe that the equation (2.5) can be transformed back into the classical lattice equation of motion:

$$\mu\ddot{y}_r = \kappa f^2(y_{r+1}-2y_r+y_{r-1}) + \kappa g_4((y_{r+1}-y_r)^3-(y_r-y_{r-1})^3).$$

This describes the original classical lattice with a renormalised linear coupling. One may as well start the analysis from this equation of motion. (We thank the referee for this comment.)

and can be easily calculated for a periodic lattice having a discrete sum over finite k' values, e.g.

$$\tfrac{1}{2}lk' = \pi n/N, \qquad n = 0, 1, 2, \ldots, N/2 \quad (N/2+1 \text{ values for } N \text{ even}).$$

Thus in the low wave number limit when $\pi n \ll N$, such that $\sin(\frac{1}{2}lk) \simeq \frac{1}{2}lk$ and for the above choice of discrete k' values; $\Sigma_{k'}\, \omega(k')$ can be estimated as approximately equal to $2(\kappa/\mu)^{1/2}(\pi/N)S_n \equiv K_n$ (constant) with $\pi n \ll N$ where S_n is the sum of first n allowed natural integers (i.e. $S_n = \frac{1}{2}n(n+1)$).

Further, in the low wave number or long wave length phonon approximation referrred to already, we may approximate ϕ and ω with IYT as:

$$\phi(k_1, k_2, k_3, k_4)$$
$$\simeq \tfrac{1}{4}\kappa g_4(\hbar/2\mu)((2\mathrm{i})^4/N)\tfrac{1}{2}lk_1 \,.\, \tfrac{1}{2}lk_2 \,.\, \tfrac{1}{2}lk_3 \,.\, \tfrac{1}{2}lk_4(\omega(k_1)\omega(k_2)\omega(k_3)\omega(k_4))^{-1/2}$$
$$\omega(k) \simeq (\kappa/\mu)^{1/2}l|\boldsymbol{k}|(1-\tfrac{1}{24}l^2k^2) = S|\boldsymbol{k}|(1-\tfrac{1}{24}l^2k^2),$$

where $S = (\kappa/\mu)^{1/2}l$; so that the equation of motion (2.5) finally becomes:

$$\ddot{y}(k,t) + S^2k^2(1-\tfrac{1}{12}l^2k^2)(1+48C_N\hbar K_n)y(k,t)$$
$$= \tfrac{1}{4}g_4S^2(l/2N)^2(2\mathrm{i})^4k \sum_{k_2,k_3,k_4} \Delta(-k+k_2+k_3+k_4)$$
$$\times k_2y(k_2,t)k_3y(k_3,t)k_4y(k_4,t). \tag{2.6}$$

Defining a new variable $u(k,t)$ and its Fourier transform

$$u(k,t) = ky(k,t), \qquad u(x,t) = N^{-1/2}\sum_k u(k,t)\exp(\mathrm{i}kx)$$

we may Fourier transform equation (2.6) into a non-linear differential equation which governing the dynamics of the lattice of anharmonicity four.

$$\frac{\partial^2}{\partial t^2}u(x,t) - S^2f^2(n,N)\frac{\partial^2}{\partial x^2}u(x,t) - \frac{1}{12}S^2l^2f^2(n,N)\frac{\partial^4}{\partial x^4}u(x,t)$$
$$-g_4S^2l^2\frac{\partial^2}{\partial x^2}(u(x,t))^3 = 0, \tag{2.7}$$

where

$$f^2(n,N) = 1 + 48C_N\hbar 2(\kappa/\mu)^{1/2}\,.\,(\pi/N)S \tag{2.7'}$$

is the frequency correction factor mentioned above. Equation (2.7) can now be converted into the KDV type by introducing the reductive perturbation techniques (Tanuiti 1974) with the following expansion and space–time rescaling:

$$u = \epsilon u^{(1)} + \epsilon^2u^{(2)} + \ldots, \qquad \xi = \epsilon(x-t), \qquad \tau = \epsilon^3 t$$

into the form

$$\frac{\partial}{\partial\xi}\left[\frac{\partial}{\partial\tau}u^{(1)} + \frac{1}{24}S^2l^2f^2(n,N)\frac{\partial^3}{\partial\xi^3}u^{(1)} + g_4\frac{S^2l^2}{2}\frac{\partial}{\partial\xi}(u^{(1)})^3\right] = 0. \tag{2.8}$$

Note that after applying this method the first integral of equation (2.8) is trivial.

Returning to the original variables, equation (2.8) now becomes

$$\frac{\partial}{\partial t}u(x,t) + S\frac{\partial}{\partial x}u(x,t) + \frac{1}{24}S^2l^2f^2(n,N)\frac{\partial^3}{\partial x^3}u(x,t) + g_4\frac{S^2l^2}{2}\frac{\partial}{\partial x}(u(x,t))^3 = 0. \tag{2.9}$$

3. Conclusion and remarks

The above is a modified KDV equation and admits one soliton solution given by (Tanuiti 1974):

$$u(x, t) = \eta \, \mathrm{sech}(a(f)(x - bst)) \tag{3.1}$$

where

$$(a(f))^2 = 2^2(3/2g_4\eta^2)(f^2(n, N))^{-1}, \qquad b = 1 + (1/4)g_4\eta^2 l^2 S, \tag{3.2}$$

with $f(n, N)$ as given by (2.7′).

Finally, it is straightforward to verify that the one soliton state is now a coherent state of excited phonons with amplitude

$$\alpha_k = (-\mathrm{i}/N^{1/2})(\mu\omega(k)/2\hbar)^{1/2}(1 + bSk/\omega(k))4^{1/2}(\eta/2a(f)lk)$$
$$\times \exp(-\mathrm{i}kbst)B(\tfrac{1}{2} + \mathrm{i}k/2a(f), \tfrac{1}{2} - \mathrm{i}k/2a(f)) \tag{3.3}$$

where $B(\alpha, \beta)$ is the β-function and enters the calculation when one defines the Fourier transform of the one soliton solution

$$u(k, t) = (N^{1/2}/L) \int_{-\infty}^{+\infty} u(x, t) \exp(-\mathrm{i}kx)\, \mathrm{d}x$$
$$= 4^{1/2}/N^{1/2} 2a(f)l \exp(-\mathrm{i}kbst)B(\tfrac{1}{2} + \mathrm{i}k/2a(f), \tfrac{1}{2} - \mathrm{i}k/2a(f)). \tag{3.4}$$

The phonon number can now be calculated by taking $|\alpha_k|^2$ from equation (3.3).

Following Ichikawa *et al* (1976), we may also estimate the mass associated with the one soliton state from the momentum equation.

$$\boldsymbol{p} = \sum_k \hbar \boldsymbol{k}\langle n_k \rangle = m(f)(1 + \tfrac{1}{4}g_4\eta^2 l^2)\boldsymbol{S}$$

where

$$m(f) \equiv \text{effective mass} = (2\eta^2/la(f))\mu. \tag{3.5}$$

Note that the frequency correction factor f enters the mass in (3.5) through the constant a. Thus we have solved the KDV equation (in the long wavelength approximation) for a lattice of anharmonicity four and have shown that the solution depends upon the correction of the oscillator frequency arising from quantum fluctuations. Now this frequency correction factor has been estimated for a periodic lattice in the low wave number limit. However, if periodicity of the lattice is not imposed, it can be seen that the summation $\Sigma_{k'} \omega(k')$ in equation (2.5′) can diverge giving rise to a divergence which is analogous to the one present in ϕ^4 theory (Rajaraman 1975). However, we have avoided this difficulty in our problem by invoking the discreteness and periodicity of our lattice system. It may be mentioned here that the factor $f(n, N)$ has been estimated in the long wavelength limit in equation (2.7′), taking only the leading power of $\tfrac{1}{2}lk'$ in the sine series occurring in $\omega(k')$. However, if there is any need higher powers of $lk'/2$ in the sine series may be retained and the correction factor (2.5′) may be re-estimated accordingly.

References

Fermi E, Pasta J R and Ulam S 1965 *Collected Papers of Enrico Fermi* vol 2 (Chicago: University of Chicago Press)
Glauber R J 1963 *Phys. Rev.* **131** 2766
Ichikawa Y H, Yajima N and Takano K 1976 *Prog. Theor. Phys.* **55** 1723
Rajaraman R 1975 *Phys. Rep.* **21**C
Tanuiti T 1974 *Prog. Theor. Phys. Suppl.* **55**
Zabusky N J 1967 *Symp. Non-linear Partial Differential Equations* ed W Ames (New York: Academic) p 233