Traveling solitons in one-dimensional quartic lattices

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We discuss the solution to classical vibrations of a one-dimensional lattice whose nearest-neighbor potential energy contains nonlinear quartic terms $V(q) \propto q^4$ in the relative displacement q. Approximate analytical solutions are derived for symmetric solitons. We derive the dispersion relation of the soliton. Solitons of odd parity are also discussed.

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I. INTRODUCTION

We discuss the solution to soliton waves on onedimensional lattices whose potential energy between adjacent atoms is

$$\mathcal{V}(r_n) = + \frac{K_4}{4} r_n^4, \quad r_n = Q_{n+1} - Q_n,$$
 (1)

where $Q_n(t)$ is the displacement of an atom at site *n*, and r_n is the relative displacement between two neighboring sites, where K_4 is constant. Earlier we found some exact analytical solutions to lattice waves with this potential.¹ Here we use approximate analytical techniques to discuss soliton waves. Our interst in solitons arises from their role in thermal transport in one-dimensional nanotubes and nanowires. We propose that solitons exist in all nonlinear lattices in one dimension, and make a significant contribution to thermal transport.

There has been much interest in solutions to waves on nonlinear lattices. The Toda lattice^{2,3} has a potential energy that is an asymmetric exponential. It has exact solutions for both soliton waves^{2–5} and lattice waves. This important result has been an impetus to finding exact solutions to excitations on other nonlinear lattices.

There have been numerous computer simulations, and analytical derivations, of the lattice dynamics of the quartic and other nonlinear lattices.^{6–28} Most of the simulations are on lattices with both quadratic and quartic interactions, and often cubic interactions. Some of these calculations found solitons. The numerical results provided the impetus for the present calculations. If a soliton does exist, then we should be able to derive a formula for it. Our calculations are for a pure quartic interaction, which reduces the number of input parameters: there is no quadratic spring constant. We have done unpublished simulations on the quartic lattice and found solitons of very narrow width—only a few lattice constants.

There have also been a few analytic calculations of solitons in lattices with quartic interactions. Kiselev^{12,13} found analytic solutions for stationary solitons. Our solutions assume the soliton is moving: solutions have the form $f(vn - \omega t)$. Other calculations assume the potential includes quadratic and perhaps cubic interactions also. Usually the analytic calculations make approximations such as the rotating-wave approximation. All of the numerical and analytical calculations find a soliton of very narrow width in real

space—at any one time only three to four atoms are actually in motion. This solution has been called the ILV for "intrinsic localized vibration."^{8,15}

Since Newton's equations have a symmetric potential, the soliton solutions have parity. We show there is one set of solutions that are symmetric, and another set that are anti-symmetric. Each of these solutions depends upon a parameter that is called v. It is related to the wave vector, or the wavelength, of the soliton wave. We derive the relationship between the frequency of the wave $\omega(v)$ and v, which gives a dispersion relation. The shape of the soliton pulse also depends upon v, but the shape does not depend upon the amplitude. Instead, the frequency is proportional to the amplitude.

II. EQUATIONS OF MOTION

The general description of classical vibrations on a onedimensional lattice assumes only interactions between first neighbors. The relative displacement of two-atom sites is called $r_n(t)$. The general equation of motion is

$$m\frac{d^2}{dt^2}r_n = K_4[r_{n+1}^3 + r_{n-1}^3 - 2r_n^3].$$
 (2)

Define a parameter τ that serves as time but has the dimensional units of inverse distance,

$$\frac{d^2}{d\tau^2}r_n = r_{n+1}^3 + r_{n-1}^3 - 2r_n^3, \quad \tau = t\sqrt{\frac{K_4}{m}}.$$
 (3)

The above equation is our primary starting point. The displacement r_n has the units of length. Write it as $r_n = a_0 R_n$, where R_n is dimensionless, while a_0 is the dimensional length. Let $s = a_0 \tau$, and get the equation

$$\frac{d^2}{ds^2}R_n = R_{n+1}^3 + R_{n-1}^3 - 2R_n^3.$$
 (4)

The length scale a_0 factors out of the equation, but is hidden in the frequency dependence. The shape of the soliton is independent of a_0 , but the frequency and velocity scale linearly with the amplitude.

III. FIRST ATTEMPT

The most obvious possible solution for a soliton is a Gaussian,



FIG. 1. Initial comparison of $F_n(x)$ and $\tilde{F}_n(x)$, as a function of x, when $v = \sqrt{3/2}$. F_n is mass times acceleration, and is given by the squares. \tilde{F}_n is the force, and is given by the circles.

$$r_n = a_0 e^{-x^2} \equiv r(x), \quad x = \upsilon n - \beta a_0 \tau, \tag{5}$$

where β gives the frequency of the wave. This function gives for the two sides of Eq. (3)

$$\frac{d^2}{d\tau^2}r_n = F_n(x) = a_0^3 \beta^2 H_2(x) e^{-x^2}, \quad H_2 = 2(2x^2 - 1), \quad (6)$$

$$\widetilde{F}_n = r(x+v)^3 + r(x-v)^3 - 2r^3(x).$$
(7)

The goal is to get a self-consistent theory by having $F_n(x) \approx \tilde{F}_n(x)$. Keep the analysis simple by setting $\beta = a_0 = 1$. Both functions are nearly equal to -2 at x=0. The function $F_n(x)$ in Eq. (6) has its maximum positive value at $x^2=3/2$. The maximum value of $\tilde{F}_n(x)$ in Eq. (7) is found near $x=v = \sqrt{3/2} = 1.224$. In Fig. 1, we compare these two functions, using that value of v, and $\beta = 1, a_0 = 1$. The two functions are quite similar in shape. No attempt here is made to make these functions more alike by selecting β . That will be done in a later section. The point is that the choice of a Gaussian is a decent approximation to a self-consistent solution. Note that the functions do not resemble each other analytically, but are similar numerically.

Since the second derivative in Eq. (6) contains the Hermite polynomial for n=2, this feature suggests that we obtain a more accurate solution using more of these functions.

IV. HERMITE POLYNOMIALS

The encouraging results of the prior section can be made more accurate by using a Hermite polynomial expansion for the displacements. The polynomials $H_n(x), x=vn-\beta a_0\tau$, are

$$H_0 = 1, \quad H_1 = 2x, \quad H_2 = 2(2x^2 - 1),$$
 (8)

$$H_3 = 4(2x^3 - 3x), \quad H_4 = 4(4x^4 - 12x^3 + 3).$$
 (9)

They are orthogonal using the Gaussian weighting factor,

$$\lambda_n \delta_{nm} = \int_{-\infty}^{\infty} dx e^{-x^2} H_n(x) H_m(x), \qquad (10)$$

$$\lambda_n = \sqrt{\pi} 2^n n!. \tag{11}$$

Using these functions, we define the displacment function in terms of a series with constant coefficients a_n ,

$$r_n = r(x) = a_0 e^{-x^2} \left[1 + \sum_{n=1}^{\infty} a_n H_n(x) \right] = a_0 R(x).$$
(12)

The two functions defined in the preceding section are

$$a_0^3 F_n(x) = \frac{d^2}{d\tau^2} r_n = a_0^3 \beta^2 e^{-x^2} \Big(H_2(x) + \sum_{n=1}^{\infty} a_n H_{n+2}(x) \Big),$$
(13)

$$\widetilde{F}_n = R^3(x+v) + R^3(x-v) - 2R^3(x).$$
(14)

These two expressions are set equal, which determines the coefficients a_n : multiply the equation by $H_{n+2}(x)$ and integrate over all values of x. Because of the orthogonality relation (10), this only makes sense if

$$0 = \int_{-\infty}^{\infty} dx H_n(x) \widetilde{F}_n(x), \quad n = 0, 1.$$
(15)

In doing this integral, we change integration variables to $y = x \pm v$ in the first two terms of \tilde{F}_n and get the integral

$$0 = \int_{-\infty}^{\infty} dy R(y)^3 G_n(y, v), \quad n = 0, 1,$$
 (16)

$$G_n(y,v) = H_n(y+v) + H_n(y-v) - 2H_n(y).$$
(17)

The function $G_n(x,v)$ does vanish for n=0,1 so that the constraint is verified. The bracket does not vanish for $n \ge 2$, which provides us with the nonlinear equations for the coefficients,

$$a_{n}\beta^{2}\lambda_{n+2} = \int_{-\infty}^{\infty} dy R(y)^{3} G_{n+2}(x,v), \qquad (18)$$

$$\beta^2 \lambda_2 = 8v^2 \int_{-\infty}^{\infty} dy R(y)^3, \qquad (19)$$

$$a_1 \beta^2 \lambda_3 = 24v^2 \int_{-\infty}^{\infty} dy R(y)^3 H_1(y),$$
 (20)

$$a_2\beta^2\lambda_4 = 16v^2 \int_{-\infty}^{\infty} dy R(y)^3 [3H_2(y) + 2v^2H_0].$$
(21)

The functions G_n are easily derived by using the generating function for Hermite polynomials,

$$\exp(2xz - z^2) = \sum_{n=0}^{\infty} H_n(x) \frac{z^n}{n!},$$
(22)

$$2e^{2xz-z^2}[\cosh(2vz)-1] = \sum_{n=0}^{\infty} G_n(x,v)\frac{z^n}{n!}.$$
 (23)

Expand the two factors on the left, $\exp(2xz-z^2)$ and $\cosh(2vz)$, in powers of z^n . Collect all terms with the same exponent of z^n , which produces G_n . This procedure works even without knowing the form of the Hermite polynomials.

We solve this set of equations with increasing accuracy. Define a parameter Λ ,

$$\beta^2 = v^2 \Lambda. \tag{24}$$

Solving these equations with increasing accuracy gives the following.

(i) Keeping only one coefficient gives, using Eq. (19) and $\lambda_2 = 8\sqrt{\pi}$,

$$\Lambda = \frac{1}{\sqrt{3}}.$$
 (25)

If we set $\beta = 1$, as we did in the previous section, then we get that $v = \sqrt[4]{3} = 1.316$, which is similar to the value ($\sqrt{3/2} = 1.224$) found in the prior section. However, there we tried to match the peak position, while here we are trying to match the moments.

(ii) Next keep two coefficients $(1, a_1)$ and find the coupled equations from Eqs. (19) and (20),

$$\sqrt{3\Lambda} = 1 + 2a_1^2,\tag{26}$$

$$a_1 \left[\sqrt{3}\Lambda = 1 + \frac{2}{3}a_1^2 \right].$$
 (27)

The solution to these equations is $a_1=0$. So the soliton seems to have a symmetric shape. Henceforth we omit antisymmetric terms—Hermite polynomials with odd integer indices. The present section is confined to symmetric solitons. Antisymmetric solitons are discussed in a later section.

(iii) Next retain $(1, a_2)$ and get the coupled equations

$$\Lambda = C_0 = \frac{1}{\sqrt{3}} \left[1 - 4a_2 + 8a_2^2 - \frac{32}{9}a_2^3 \right],$$
 (28)

$$24\Lambda a_2 = 2v^2 C_0 + 3C_2, \tag{29}$$

$$C_n = \sqrt{\frac{1}{\pi}} \int dx R(x)^3 H_n(x), \qquad (30)$$

$$C_2 = \frac{1}{\sqrt{3}} \left[-\frac{4}{3} + 8a_2 - \frac{32}{3}a_2^2 + \frac{320}{27}a_2^3 \right].$$
 (31)

There are two equations and three unknowns: a_2 , v^2 , and Λ : note that Λ gives the frequency β . One variable is a free parameter. The most obvious choice is v, which is related to the wavelength of the soliton. While that is obvious physically, numerically the best choice is a_2 . This choice makes



FIG. 2. Graph of v^2 and β^2 as a function of a_2 .

the equations simple to solve. After selecting a_2 , then $C_{0,2}$ are both known. Then we get

$$\Lambda = C_0, \tag{32}$$

$$v^2 = 12\alpha_2 - \frac{3C_2}{2C_0},\tag{33}$$

and β^2 is found from Eq. (24). Figure 2 shows the resulting values for v^2 and β^2 . Better values are given below, but here we wish to show the type of result. It is clear that v^2 can vanish around $a_2 \approx -0.2$, and physical values must have a_2 greater than this value. At small values of v, the soliton is spread out, while at larger values of v it is localized to a few lattice points at any time.

Adding the parameter a_2 does not improve the type of agreement that is illustrated in Fig. 1. Instead, this parameter provides a change in the shape of the soliton.

(iv) Next we keep five even coefficients $(1, a_2, a_4, a_6, a_8)$. The relevant equations are the set above plus three more,

$$R(x) = e^{-x^2} [1 + a_2 H_2(x) + a_4 H_4(x) + a_6 H_6(x) + a_8 H_8(x)],$$

$$\Lambda = C_0, \tag{34}$$

$$24\Lambda a_2 = 2v^2 C_0 + 3C_2, \tag{35}$$

$$10(24)^2 \Lambda a_4 = 16v^4 C_0 + 60v^2 C_2 + 15C_4, \qquad (36)$$

$$8(8!)\Lambda a_6 = 16v^6 C_0 + 112v^4 C_2 + 70v^2 C_4 + 7C_6, \quad (37)$$

$$128(10!)\Lambda a_8 = 256v^8C_0 + 2880v^6C_2 + 3360v^4C_4 + 840v^2C_6 + 45C_8.$$
(38)

There are five equations and six unknowns. Note that the parameters C_n depend upon (a_2, a_4, a_6, a_8) . Again let a_2 be the independent variable. Eliminate Λ using Eq. (34), and eliminate v^2 using Eq. (35). There remain three equations in terms of the three unknowns (a_4, a_6, a_8) . For example, Eq. (36) is now

TABLE I. Properties of the symmetric soliton.

<i>a</i> ₂	a_4	<i>a</i> ₆	v^2	β^2
-0.22	0.02414	-0.00176	0.0366	0.0911
-0.21	0.02200	-0.00153	0.1397	0.3158
-0.20	0.01991	-0.00132	0.2416	0.4967
-0.18	0.01600	-0.00094	0.4414	0.7542
-0.16	0.01238	-0.00063	0.6333	0.9091
-0.14	0.00913	-0.00038	0.8163	0.9952
-0.12	0.00627	-0.00019	0.9888	1.0378
-0.10	0.00383	-0.00006	1.1512	1.0544
-0.08	0.00180	0.00003	1.3052	1.0567
-0.06	0.00014	0.00009	1.4531	1.0520
-0.04	-0.00117	0.00011	1.5975	1.0449
-0.02	-0.00213	0.00010	1.7407	1.0381
0.00	-0.00274	0.00008	1.8846	1.0332
0.02	-0.00298	0.00003	2.0307	1.0308
0.04	-0.00283	-0.00002	2.1799	1.0311
0.06	-0.00230	-0.00007	2.3324	1.0337
0.08	-0.00139	-0.00011	2.4882	1.0378
0.10	-0.00008	-0.00014	2.6462	1.0427
0.12	0.00160	-0.00014	2.8048	1.0476
0.14	0.00368	-0.00012	2.9609	1.0513

$$a_4 = \frac{2}{5}a_2^2 + \frac{a_2}{40}\left(\frac{C_2}{C_0}\right) - \frac{3}{320}\left(\frac{C_2}{C_0}\right)^2 + \frac{C_4}{384C_0}.$$
 (39)

This equation is nonlinear, since the right-hand side also depends on a_4 through the parameters C_n . Yet we found it could be solved easily by iteration. Note that it only depends on the parameters a_n . Start with the selected value of a_2 and initially $a_4=0$, $a_6=0$, $a_8=0$. After finding (a_4, a_6, a_8) , we find v^2 using Eq. (33).

The parameters (a_4, a_6, a_8) are a slave to a_2 , and serve to improve the self-consistency of the type of comparison shown in Fig. 1. Additional parameters $(a_{10}, ...)$ are also slaves to a_2 , and should increase the accuracy of the series.

Table I gives a list of the various parameters as a function of a_2 for the symmetric soliton. We did not include a_8 , but it also of order $O(10^{-4})$. Note that v^2 has a monotonic dependence on a_2 . In the region where $v^2 \rightarrow 0$, the curve is quite linear. The data for $\beta(v)$ are graphed in Fig. 3. The parameter v is related to the wave vector. If a is the lattice constant, then the distance is y=an. If v=ka, then $x=ky-\omega t$, where

$$\omega = \beta a_0 \sqrt{\frac{K_4}{m}}.$$
 (40)

The phase velocity is $v_p = \omega/k \propto \beta/v$, and the constant value is given in Eq. (24).

We solved these coefficients by adding one coefficient at a time. The results for the symmetric soliton seem to be converging as we add more terms to the series of Hermite polynomials in Eq. (12). When we added a_8 , the results changed



FIG. 3. Symmetric soliton dispersion $\beta(v)$.

by less than 1%. Note in Table I the small values of $a_4 \sim 10^{-2}$, $a_6 \sim 10^{-4}$. The series seems to converge to a reasonable result.

The soliton dispersion resembles many phonon-dispersion curves. It rises linearly at small values of v, and then levels off around $v \sim 1$. After that, it makes only small changes with v. Each additional term in the series for a_n seems to flatten this upper portion of the dispersion curve, and to bring β closer to 1.

Figure 1 shows the initial comparison of the two force functions F_n , \tilde{F}_n . In Fig. 4, we compare them again, but now using our fiveterm series in Eq. (12). For comparison, we selected the values for $a_2=0$. It provides an average result. The two curves are more alike for $a_2>0$, and less alike for increasingly negative values of a_2 . Now the two curves agree to about 1% or 2% over the full range of x values. Such agreement is expected when we require their first eight moments to be equal.



FIG. 4. A comparison of the two force terms for the case in which $a_2=0$, v=1.375. The function F_n is the second derivative of r_n , and is given by the squares. The function \tilde{F}_n is the force, and is given by the circles.

V. ANTISYMMETRIC SOLITONS

The initial Eq. (3) has a symmetric potential. That suggests the solutions have parity. They are either purely even or purely odd. The prior section gave the even solutions. Here we give the odd solutions.

We suppose there is a solution of the form

$$r_n = r(x) = a_0 e^{-x^2} [H_1(x) + a_3 H_3(x) + a_5 H_5(x) + \cdots],$$
(41)

$$\frac{d^2}{d\tau^2}r_n = \beta^2 a_0^3 e^{-x^2} [H_3(x) + a_3 H_5(x) + a_5 H_7(x) + \cdots],$$
(42)

$$=a_0^3 F_n, (43)$$

$$\tilde{F}_n = R(x+v)^3 + R(x-v)^3 - 2R(x)^3.$$
(44)

Again we find equations for the coefficients $(a_3, a_5, ...)$ by setting $F_n = \tilde{F}_n$ and taking moments

$$\beta^{2}\lambda_{3} = 24v^{2} \int dx R(x)^{3} H_{1}(x), \qquad (45)$$

$$\beta^2 a_3 \lambda_5 = 80v^2 \int dx R(x)^3 [2v^2 H_1(x) + H_3], \qquad (46)$$

$$\beta^2 a_5 \lambda_7 = 56v^2 \int dx R(x)^3 [16v^4 H_1(x) + 20v^2 H_3 + 3H_5],$$
(47)

$$\beta^2 a_7 \lambda_9 = 96v^2 \int dx R(x)^3 \times [48v^6 H_1(x) + 112v^4 H_3 + 42v^2 H_5 + 3H_7].$$
(48)

The integrals can be evaluated in terms of the constants C_n ,

$$2\Lambda = C_1, \tag{49}$$

$$48a_3\Lambda = 2v^2C_1 + C_3, \tag{50}$$

$$11520a_5\Lambda = 16v^4C_1 + 20v^2C_3 + 3C_5, \tag{51}$$

$$48(8!)a_7\Lambda = 48v^6C_1 + 112v^4C_3 + 42v^2C_5 + 3C_7.$$
 (52)

Equations (49) and (50) are solved for Λ, v^2 and the results are inserted into Eqs. (51) and (52). These equations depends only on (a_3, a_5, a_7) . After selecting a value for a_3 , the results for a_5, a_7 are found by iteration.

This process did not converge as well as the similar calculation for the symmetric soliton. This slow convergence has several possible explanations: (i) solutions exist but the series converges slowly, or (ii) the solutions do not actually exist. At the moment we are undecided between these two scenerios, but lean toward (ii). Figure 5 shows the dispersion



FIG. 5. The dispersion curve $\beta(v)$ of the antisymmetric soliton as given by two series. The squares have the terms with (a_3, a_5) , while the red circles have the terms (a_3, a_5, a_7) .

curve $\beta(v)$ obtained in the last two iterations. One curve has (a_3, a_5) while the other has (a_3, a_5, a_7) . The results change substantially. Actually, before submitting this manuscript, we also modified the computer code to include the next term $a_9H_9(x)$. Values of $a_9 \sim O(10^{-5})$. However, the dispersion curve $\beta(v)$ of Fig. 5 changed further, adding another curve much further to the left of those already in this figure. The series does not seem to be converging. We concluded that there are no stable antisymmetric solutions.

Kiselev^{12,13} also consider solitons on the quartic lattice. He considered only stationary solutions, whereas we consider only moving solutions. That may explain the different answers, since he found stable symmetric and stable antisymmetric solutions. He also calculated the dispersion curve for a soliton on a lattice with two different, alternating, masses, but did not present the dispersion curve for a lattice with a single mass.

There have been other reports of symmetric and antisymmetric solitons on lattices with both quadratic and quartic interactions.^{24–26} The quadratic interaction seems to stabilze the antisymmetric solutions. Incidently, the words symmetric and antisymmetric must be used carefully, with regard to the variable. A soliton that is symmetric with respect to the lattice displacement Q_n is antisymmetric with respect to the relative displacement $r_n = Q_{n+1}, -Q_n$, and vice versa. Our results find symmetric solitons with respect to the relative displacement.

VI. DISCUSSION

Solitons are solitary waves that can travel without damping along a one-dimensional chain of atoms with nonlinear potential energy between neighboring atoms. Here we have determined the properties of the soliton on a lattice that has a quartic interaction between displacements of first neighbors. Since the equations of motion are unchanged by a parity operation, we found that the solutions had either even or odd parity. We considered separately the solutions with even, and with odd, parity.

The solutions with even parity were obtain with an accuracy that was near 1%. We showed the relative displacements r_n could be expanded in a power series of Hermite polynomials,

$$r_n(t) = a_0 e^{-x^2} [1 + a_2 H_2(x) + a_4 H_4(x) + a_6 H_6(x) + \cdots],$$
(53)

$$x = vn - \beta a_0 \tau. \tag{54}$$

The overall dimensional constant a_0 factors out of the equations, and has no contribution to the shape of the soliton. It does determine the frequency of the soliton, and its velocity. We determined the solution including the other four coefficients (a_2, a_4, a_6, a_8) . The displacement is written as a function of $x=vn-\omega t$, $\omega=\beta a_0\sqrt{K_4/m}$. The soliton shape and frequency depended upon the wavelength parameter v. This behavior is identical to that of the soliton in the Toda lattice, where Toda wrote his solution as $x=\mu n-\beta \tau$, where τ is a dimensionless time. His solutions $\beta(\mu)$ also depended upon μ .

The major results are shown in Figs. 3 and 4. Figure 3 shows the soliton dispersion $\beta(v)$. Figure 4 shows the consistency obtained in the solution. One curve is the left-hand side of Newton's law, while the other curve is the right-hand

side. The agreement is on the order of 1%. Improved agreement could be obtained by adding more terms to the series in Eq. (53). In general, we think our series solution is converging to a good description of the soliton for the quartic lattice.

Our experience was much less successful for the antisymmetric solutions, where r(x) has odd parity. We took solutions of the form

$$r_n(t) = a_0 e^{-x^2} [H_1(x) + a_3 H_3(x) + a_5 H_5(x) + a_7 H_7(x) + \cdots].$$
(55)

A set of nonlinear equations was found for the unknown coefficients $(a_3, a_5, a_7, ...)$ as a function of v. However, when solving these equations, the answers did not converge. They change completely every time a new term is added to the series. Perhaps there is no soliton of odd parity.

A graph of r(x) appears as a Gaussian, for every value of v. We do not provide a graph since it is dull. A more interesting curve is to graph $r_n(t)$ as a function of lattice site n. For most values of $v \sim O(1)$, only three or four points are "nonzero." By nonzero, we mean larger than 0.01 when $a_0 = 1$. So the soliton is quite local, and at any time, only a few sites are displaced from zero.

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