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Integrability of Low Particle-number Models for Solids

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Abstract

We introduce a model Hamiltonian that describes, for different choices of the parameters, simple anharmonic models for a solid. We have applied the Painlevé test to identify integrable and non-integrable cases. In the integrable cases the identification has been confirmed by deriving explicit expressions for the additional conserved quantities. The analysis demonstrates the sensitivity of lattice integrability to both the order of the anharmonicity and the nature of the boundary conditions.

1. Introduction

Equipartition of energy is a fundamental property of crystals. If energy is supplied to (or subtracted from) a crystal then eventually the energy will be redistributed uniformly among all the degrees of freedom. One consequence of this property is that the specific heat of a crystal can be obtained simply by counting the number of degrees of freedom and assigning equal portions of energy to each degree of freedom. Consider the harmonic lattice model for a solid. This system, which consists of N atoms in a three-dimensional lattice with linear interatomic forces, is equivalent to a set of $3N$ uncoupled harmonic oscillators. Since there are $6N$ degrees of freedom (one potential energy and one kinetic energy per oscillator) the specific heat is simply:

$$C_v = 6N(\tfrac{1}{2}k_b)\,. \tag{1}$$

This is the well known Dulong–Petit Law and is well confirmed by experiments (at least at temperatures where the classical approximation is valid, Ashcroft and Mermin 1976). However, from a theoretical viewpoint the situation is less clear; equipartition of energy cannot occur in the harmonic lattice model. Uncoupled oscillators cannot redistribute energy among themselves. It is therefore supposed that there are anharmonic forces present that allow energy exchanges among the modes resulting in equipartition of energy.

In more general terms, the harmonic lattice model is an integrable system. Equipartition of energy is not possible in integrable systems due to the presence of additional conservation laws that cause the energy to become trapped in some of the degrees of freedom and frozen out of others. In the harmonic lattice the fundamental modes are phonons and the phonon energies

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are conserved. The inclusion of anharmonic terms is a necessary but not sufficient condition for non-integrability. For example, the one-dimensional Toda (1981) lattice is an anharmonic but integrable model; the fundamental modes are solitons and the soliton energies are conserved.

In the present paper we examine the integrability properties of some very simple one-dimensional anharmonic lattice models. In Section 2 we introduce a model Hamiltonian that includes, as special cases, four-particle clamped chains and three-particle periodic chains with quadratic and/or cubic interatomic forces in addition to the linear forces. In Section 3 we apply the strong Painlevé test and the weak Painlevé test to decide which of these cases is integrable. We calculate the additional conserved quantities explicitly for the integrable cases in Section 4. Finally in Section 5 we discuss the sensitivity of integrability to both the order of the anharmonicity and the nature of the boundary conditions.

2. One-dimensional Models for Solids

The simplest one-dimensional model for a solid consists of a chain of atoms coupled by nearest neighbour interatomic forces that are a function of the relative displacements of the atoms from their equilibrium sites. In general the interatomic potential can be Taylor expanded in powers of the relative displacements. In the following, x_n denotes the displacement of the nth atom from its equilibrium site and λ_m are force constants. Two types of boundary conditions are investigated:

(i) Clamped end boundary conditions ($x_0 = x_{N+1} = 0$). The Hamiltonian is

$$\mathcal{H} = \sum_{n=0}^{N} \left(\tfrac{1}{2}\dot{x}_n^2 + \tfrac{1}{2}(x_{n+1} - x_n)^2 + \sum_{m=3}^{\infty} \frac{\lambda_m}{m}(x_{n+1} - x_n)^m \right). \tag{2}$$

If λ_m is nonzero for some m in the sum to infinity then the model is nonlinear. In the absence of the nonlinear terms the normal mode coordinates

$$x_n = \left(\frac{2}{N+1}\right) \sum_{s=1}^{N} a_s \sin\left(\frac{n\pi s}{N+1}\right), \qquad s = 1, 2, \ldots, N, \tag{3}$$

with frequencies

$$\omega_s = 2\sin\left(\frac{s\pi}{2(N+1)}\right), \tag{4}$$

separate the Hamiltonian into a sum of independent harmonic oscillators. The full nonlinear Hamiltonian can be expressed in terms of the normal mode coordinates by using identities (A1) and (A2) in the Appendix:

$$\begin{aligned} \mathcal{H} &= \tfrac{1}{2}\sum_{s=1}^{N} \dot{a}_s^2 + \tfrac{1}{2}\sum_{s=1}^{N} a_s^2\, \omega_s^2 \\ &\quad + \sum_{m=3}^{\infty} \frac{\lambda_m}{m}[2(N+1)]^{-m/2} \sum_{s_1=\pm 1, \ldots, s_m=\pm 1}^{\pm N} a_{s_1} \ldots a_{s_m}\, \omega_{s_1} \ldots \omega_{s_m}\, K_{s_1+\ldots+s_m}, \end{aligned} \tag{5}$$

where

$$K_{s_1+\ldots+s_m} = \begin{cases} +(N+1) & \text{if } s_1+\ldots+s_m = 2q(N+1) \quad \text{with } q = 0, \pm 2, \pm 4, \ldots, \\ -(N+1) & \text{if } s_1+\ldots+s_m = 2q(N+1) \quad \text{with } q = \pm 1, \pm 3, \ldots, \\ 0 & \text{otherwise}. \end{cases} \tag{6}$$

(ii) Periodic boundary conditions ($x_n = x_{N+n}$). The Hamiltonian is

$$\mathcal{H} = \sum_{n=1}^{N} \left(\tfrac{1}{2}\dot{x}_n^2 + \tfrac{1}{2}(x_{n+1}-x_n)^2 + \sum_{m=3}^{\infty} \frac{\lambda_m}{m}(x_{n+1}-x_n)^m \right). \tag{7}$$

In this case suitable normal mode coordinates are

$$x_n = \sqrt{\frac{1}{N}} \sum_s a_s \exp\left(\frac{\mathrm{i}2\pi sn}{N}\right) \qquad s = 0, \pm 1, \pm 2, \ldots \pm\left(\frac{N}{2}-1\right), \frac{N}{2} \qquad N \text{ even}$$

$$s = 0, \pm 1, \pm 2, \ldots \pm\left(\frac{N-1}{2}\right) \qquad N \text{ odd}, \tag{8}$$

with frequencies

$$\omega_s = 2\sin\left(\frac{s\pi}{N}\right). \tag{9}$$

The a_s are complex with $a_{-s} = a_s{}^*$. The nonlinear Hamiltonian is written in terms of the normal mode transformation by using identities (A3) and (A4) in the Appendix:

$$\begin{aligned} \mathcal{H} &= \tfrac{1}{2}\sum_s |\dot{a}_s|^2 + \tfrac{1}{2}\sum_s |a_s|^2\omega_s^2 \\ &\quad + \sum_{m=3}^{\infty} \frac{\lambda_m}{m}\left(\frac{\mathrm{i}}{\sqrt{N}}\right)^m \sum_{s_1,\ldots,s_m} a_{s_1}\ldots a_{s_m}\,\omega_{s_1}\ldots\omega_{s_m} J_{s_1+\ldots+s_m}, \end{aligned} \tag{10}$$

where

$$J_{s_1+\ldots+s_m} = \begin{cases} +N & \text{if } s_1+\ldots+s_m = qN \quad \text{with } q = 0, \pm 2, \pm 4, \ldots, \\ -N & \text{if } s_1+\ldots+s_m = qN \quad \text{with } q = \pm 1, \pm 3, \ldots, \\ 0 & \text{otherwise}. \end{cases} \tag{11}$$

If the nearest neighbour relative displacements are small then the high order nonlinear terms may be neglected to a good approximation. Terms above fourth order are neglected in the following. Starting with the Hamiltonians in equations (5) and (10) it is an easy matter to derive the two special cases:

(I) Four-particle clamped cubic ($\lambda_3 \neq 0$) plus quartic ($\lambda_4 \neq 0$) chain; $N = 2$, $m = 3, 4$:

$$\mathcal{H} = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) + \tfrac{1}{2}(x^2 + 3y^2) + \frac{\lambda_3}{\sqrt{2}}(x^2y - y^3) + \frac{\lambda_4}{8}(6x^2y^2 + x^4 + 9y^4), \tag{12}$$

where $x = a_1$ and $y = a_2$.

(II) Three-particle periodic cubic ($\lambda_3 \neq 0$) plus quartic ($\lambda_4 \neq 0$) chain; $N = 3$, $m = 3, 4$:

$$\mathcal{H} = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) + \tfrac{1}{2}(x^2 + y^2) + \frac{\lambda_3}{3}(3x^2y - y^3) + \frac{3\lambda_4}{4}(x^4 + 2x^2y^2 + y^4), \tag{13}$$

where $x=(a_1+a_1^*)/2$, $y=(a_1^*-a_1)/2i$ and the energy has been rescaled by a factor 1/6.

The pure cubic and pure quartic cases are obtained by setting $\lambda_3=0$ and $\lambda_4=0$ respectively.

We now consider a slightly more general Hamiltonian that includes the above physically distinct cases for different choices of the parameters A, B, C, D, E, F, G:

$$\mathcal{H} = \tfrac{1}{2}(\dot{x}^2+\dot{y}^2)+\tfrac{1}{2}(Ax^2+By^2)+Dx^2y-\frac{C}{3}y^3+\tfrac{1}{4}(Ex^4+2Fx^2y^2+Gy^4). \tag{14}$$

The corresponding Hamilton–Jacobi equations of motion are

$$\ddot{x} = -Ax-2Dxy-Ex^3-Fxy^2, \tag{15a}$$

$$\ddot{y} = -By-Dx^2+Cy^2-Fx^2y-Gy^3. \tag{15b}$$

In the following we determine those values of $A, B, \ldots, G$ ($E\neq 0$, $F\neq 0, G\neq 0$) for which the above system is strong Painlevé-type or weak Painlevé-type (see definitions below). Additional constants of the motion are explicitly derived for these cases, thus establishing integrability. Painlevé analysis has been carried out previously for two special cases of the Hamiltonian in (14): (i) the generalised Henon–Heiles (1964) Hamiltonian $G=F=E=0$ (Bountis *et al.* 1982; Chang *et al.* 1982); (ii) the generalised quartic Hamiltonian $D=C=0$ (Bountis *et al.* 1982; Lakshmanan and Sahadevan 1985). More recently, Yoshida *et al.* (1988) investigated the case of $B=A$, $G=F=E$. They used a theorem of Ziglin to prove non-integrability except when (i) $D=C=0$, (ii) $D=-C/3$, $E=2C^2/9A$, (iii) $D=-C/2$ and (iv) $D=C$, $E=2C^2/9A$. We will refer to these exceptional cases as non Z-type.

3. Painlevé Analysis

A system of ordinary differential equations can be classified according to the nature of its singularities in the complex time plane as follows:

(i) Strong Painlevé-type (Ablowitz *et al.* 1980). The solution in the neighbourhood of an arbitrary movable singularity t_0 can be expressed as an expansion in powers of $(t-t_0)^{-n}$, where n is an integer determined solely from the leading order.

(ii) Weak Painlevé-type (Ramani *et al.* 1982). The solution in the neighbourhood of an arbitrary movable singularity t_0 can be expressed as an expansion in powers of $(t-t_0)^{-1/n}$, where n is a nonzero positive integer that depends solely on the leading-order behaviour of the singularity.

It is widely conjectured that systems that are (non) Painlevé-type are also (non) integrable (see e.g. the reviews by Steeb *et al.* 1985; Yoshida *et al.* 1987; Ramani *et al.* 1989). In the following we use the abbreviation P-type to denote Painlevé-type. The general method for Painlevé analysis consists of a three step algorithm that is well described in the above reviews.

Step 1. Leading-order Behaviour

Substitute the leading-order ansatz

$$x=a_0\,\tau^{\alpha}, \quad y=b_0\,\tau^{\beta}, \quad \tau=(t-t_0); \quad \alpha,\beta<0, \tag{16}$$

into the equations of motion to obtain the leading-order equations

$$a_0\,\alpha(\alpha-1)\tau^{\alpha-2} = -Ea_0^3\,\tau^{3\alpha} - Fa_0\,b_0^2\,\tau^{\alpha+2\beta}, \tag{17a}$$

$$b_0\,\beta(\beta-1)\,\tau^{\beta-2} = -Fa_0^2\,b_0\,\tau^{2\alpha+\beta} - Gb_0^3\,\tau^{3\beta}. \tag{17b}$$

There are three distinct cases to consider: Case 1, $\alpha=\beta$; Case 2, $\alpha<\beta$; and Case 3, $\beta<\alpha$. The exponents and coefficients of the leading-order behaviours for each case are listed below. In the following, $\lambda=F/E$ and $\kappa=F/G$.

Case 1

$$\alpha=-1,\quad \beta=-1,\qquad a_0^2=\frac{2}{E}\left(\frac{\kappa-1}{1-\lambda\kappa}\right),\qquad b_0^2=\frac{2}{G}\left(\frac{\lambda-1}{1-\lambda\kappa}\right),$$

$$\ddot{x}=-Ex^3-Fxy^2,\quad \ddot{y}=-Fx^2y-Gy^3. \tag{18}$$

Case 2(i)

$$\alpha=-1,\quad \beta=\tfrac{1}{2}[1+(1+8\lambda)^{\frac{1}{2}}],\qquad a_0^2=-\frac{2}{E},\quad b_0^2\ \text{arbitrary},$$

$$\ddot{x}=-Ex^3,\quad \ddot{y}=-Fx^2y. \tag{19}$$

Case 2(ii)

$$\alpha=-1,\quad \beta=\tfrac{1}{2}[1-(1+8\lambda)^{\frac{1}{2}}],\qquad a_0^2=-\frac{2}{E},\quad b_0^2\ \text{arbitrary},$$

$$\ddot{x}=-Ex^3,\quad \ddot{y}=-Fx^2y. \tag{20}$$

Case 3(i)

$$\alpha=\tfrac{1}{2}[1+(1+8\kappa)^{\frac{1}{2}}],\quad \beta=-1,\qquad a_0^2\ \text{arbitrary},\quad b_0^2=-\frac{2}{G},$$

$$\ddot{x}=-Fxy^2,\quad \ddot{y}=-Gy^3. \tag{21}$$

Case 3(ii)

$$\alpha=\tfrac{1}{2}[1-(1+8\kappa)^{\frac{1}{2}}],\quad \beta=-1,\qquad a_0^2\ \text{arbitrary},\quad b_0^2=-\frac{2}{G},$$

$$\ddot{x}=-Fxy^2,\quad \ddot{y}=-Gy^3. \tag{22}$$

From the above analysis we deduce that the most singular behaviour that is supported is τ^{-1}.

Step 2. Resonances

We now look for an expansion about the leading-order term by substituting the resonance ansatz

$$x=a_0\,\tau^{\alpha}+p\,\tau^{\alpha+r},\qquad y=b_0\,\tau^{\beta}+q\,\tau^{\beta+r} \tag{23}$$

into the leading-order equations (17) and retaining only those terms that are linear in p and q. The resonance equations for the different cases are listed below.

Case 1

Resonance equation

$$\begin{pmatrix} (r-1)(r-2)+3Ea_0^2+Fb_0^2 & 2Fa_0 b_0 \\ 2Fa_0 b_0 & (r-1)(r-2)+3Gb_0^2+Fa_0^2 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \tag{24}$$

This will hold for arbitrary p, q if the determinant of the matrix vanishes. Resonances occur at

$$r=-1, \quad 4, \quad \tfrac{3}{2} \pm \tfrac{1}{2}\left\{9+16\left(\frac{\kappa+\lambda-1-\kappa\lambda}{\kappa\lambda-1}\right)\right\}^{\frac{1}{2}} . \tag{25}$$

The resonance at $r=-1$ corresponds to the arbitrariness of t_0. For P-type we require three additional non-negative integer resonances. There are clearly two possibilities:

$$r=-1, 0, 3, 4 \qquad \frac{\kappa+\lambda-1-\kappa\lambda}{\kappa\lambda-1}=0 ; \tag{26}$$

$$r=-1, 1, 2, 4 \qquad \frac{\kappa+\lambda-1-\kappa\lambda}{\kappa\lambda-1}=-\tfrac{1}{2} . \tag{27}$$

The above cases are called main branches. There are other cases where there are only two additional non-negative integer resonances. These cases, called subsidiary branches (Lakshmanan and Sahadevan 1985), will not be discussed here.

Case 2

Resonance equation

$$\begin{pmatrix} (r-1)(r-2)-6 & 0 \\ -2Fa_0 b_0 & r^2+2r\beta-r \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \tag{28}$$

Resonances occur at

$$r=0, \ -1, \ 1-2\beta, \ 4 . \tag{29}$$

Case 2(i)

$$\beta=\tfrac{1}{2}+\tfrac{1}{2}(1+8\lambda)^{\frac{1}{2}} . \tag{30}$$

In order that we have a sufficient number of positive integer resonances we require $1-2\beta>0$, i.e. $\beta<1/2$; however, this is not allowed in this case.

Case 2(ii)

$$\beta=\tfrac{1}{2}-\tfrac{1}{2}(1+8\lambda)^{\frac{1}{2}} . \tag{31}$$

Once again we require $1-2\beta$ to be a positive integer. We also require $\beta > -1$ to be consistent with our earlier analysis (see the remark at the end of step 1). There are two possibilities:

$$r = -1, 0, 1, 4 \qquad \beta = 0, \quad \lambda = 0\,; \tag{32}$$

$$r = -1, 0, 2, 4 \qquad \beta = -\tfrac{1}{2}, \quad \lambda = \tfrac{3}{8}\,. \tag{33}$$

We reject the case corresponding to $\lambda = 0$ since we assumed at the outset that F was nonzero.

Case 3

The symmetry between x and y variables in leading-order terms allows us to deduce the result immediately from Case 2. In particular we have one possibility to consider analogous to Case 2(ii):

$$r = -1, 0, 2, 4 \qquad \alpha = -\tfrac{1}{2}, \quad \kappa = \tfrac{3}{8}\,. \tag{34}$$

Step 3. Arbitrary Constants

We now derive recursion relations for the coefficients in the Laurent series by substituting

$$x = \sum_{j=0}^{\infty} a_j (t-t_0)^{j+\alpha}\,, \qquad y = \sum_{j=0}^{\infty} b_j (t-t_0)^{j+\beta} \tag{35}$$

into the full equations of motion (15) and equating coefficients of equal powers. In this way we verify whether the Laurent series has a sufficient number of arbitrary constants without the need to introduce logarithmic terms. After some algebra we find the following recursion relations:

Case 1

a_0:

$$E a_0^2 + F b_0^2 = -2\,, \qquad F a_0^2 + G b_0^2 = -2\,. \tag{36a, b}$$

a_1:

$$\begin{pmatrix} 2Ea_0^2 - 2 & 2Fa_0\, b_0 \\ 2Fa_0\, b_0 & 2Gb_0^2 - 2 \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} -2Da_0\, b_0 \\ -Da_0^2 + Cb_0^2 \end{pmatrix}. \tag{37}$$

a_j, b_j ($j \geq 2$):

$$\begin{aligned} [(j-1)(j-2) + 3Ea_0^2 + Fb_0^2]a_j + [2Fa_0\, b_0]b_j &= \\ &-Aa_{j-2} - 2D\sum_{k=0}^{j-1} a_{j-k-1}\, b_k - E\sum_{k=1}^{j-1} a_0\, a_{j-k}\, a_k \\ &-E\sum_{l=1}^{j-1}\sum_{k=0}^{l} a_{j-l} a_{l-k}\, a_k - F\sum_{k=1}^{j-1} a_0\, b_{j-k}\, b_k \\ &-F\sum_{l=1}^{j-1}\sum_{k=0}^{l} a_{j-l}\, b_{l-k}\, b_k\,, \end{aligned} \tag{38a}$$

$$[2Fa_0 b_0]a_j + [(j-1)(j-2) + 3Gb_0^2 + Fa_0^2]b_j = -Bb_{j-2} - D\sum_{k=0}^{j-1} a_{j-k-1}\,a_k + C\sum_{k=0}^{j-1} b_{j-k-1}\,b_k - F\sum_{k=1}^{j-1} a_0\,a_{j-k}\,b_k - F\sum_{l=1}^{j-1}\sum_{k=0}^{l} a_{j-l}\,a_{l-k}\,b_k - G\sum_{k=1}^{j-1} b_0\,b_{j-k}\,b_k - G\sum_{l=1}^{j-1}\sum_{k=0}^{l} b_{j-l}\,b_{l-k}\,b_k\,. \qquad (38b)$$

Case 2

a_0, b_0:

$$2a_0 = -Ea_0^3, \qquad \tfrac{3}{4}b_0 = -Fa_0^2\,b_0\,. \qquad (39a, b)$$

a_1, b_1:

$$\begin{pmatrix} 3Ea_0^2 & 0 \\ 2Fa_0\,b_0 & Fa_0^2 - \frac{1}{4} \end{pmatrix}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} -Fb_0^2\,a_0 \\ -Gb_0^3 \end{pmatrix} \qquad (40)$$

a_j, b_j $(j \geq 2)$:

$$[(j-1)(j-2) + 3Ea_0^2]a_j = -Aa_{j-2} - E\sum_{k=1}^{j-1} a_0\,a_{j-k}\,a_k - E\sum_{l=1}^{j-1}\sum_{k=0}^{l} a_{j-l}\,a_{l-k}\,a_k - F\sum_{l=0}^{j-1}\sum_{k=0}^{l} a_{j-1-l}\,b_{l-k}\,b_k\,, \qquad (41a)$$

$$[2Fa_0\,b_0]a_j + [(j-\tfrac{1}{2})(j-\tfrac{3}{2}) + Fa_0^2]b_j = -Bb_{j-2} - G\sum_{l=0}^{j-1}\sum_{k=0}^{l} b_{j-1-l}\,b_{l-k}\,b_k - F\sum_{k=1}^{j-1} a_0\,a_{j-k}\,b_k - F\sum_{l=1}^{j-1}\sum_{k=0}^{l} a_{j-l}\,a_{l-k}\,b_k\,. \qquad (41b)$$

Case 3

a_0, b_0:

$$\tfrac{3}{4}a_0 = -Fa_0\,b_0^2, \qquad 2b_0 = -Gb_0^3\,. \qquad (42a, b)$$

a_1, b_1:

$$\begin{pmatrix} -\frac{1}{4} + Fb_0^2 & 2Fa_0\,b_0 \\ 0 & 3Gb_0^2 \end{pmatrix}\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} -2Da_0\,b_0 - Ea_0^3 \\ Cb_0^2 - Fa_0^2\,b_0 \end{pmatrix}. \qquad (43)$$

a_j, b_j $(j \geq 2)$:

$$[(j-\tfrac{1}{2})(j-\tfrac{3}{2}) + Fb_0^2]a_j + [2Fa_0\,b_0]b_j = -Aa_{j-2} - 2D\sum_{k=0}^{j-1} a_{j-1-k}\,b_k - E\sum_{l=0}^{j-1}\sum_{k=0}^{l} a_{j-1-l}\,a_{l-k}\,a_k - F\sum_{k=1}^{j-1} a_0\,b_{j-k}\,b_k - F\sum_{l=1}^{j-1}\sum_{k=0}^{l} a_{j-l}\,b_{l-k}\,b_k\,, \qquad (44a)$$

$$[(j-1)(j-2)+3Gb_0^2]b_j = -Bb_{j-2}-D\sum_{k=0}^{j-2} a_{j-2-k}\,a_k+C\sum_{k=0}^{j-1} b_{j-1-k}\,b_k-F\sum_{l=0}^{j-1}\sum_{k=0}^{l} a_{j-1-l}\,a_{l-k}\,b_k$$
$$-G\sum_{k=1}^{j-1} b_0\,b_{j-k}\,b_k-G\sum_{l=1}^{j-1}\sum_{k=0}^{l} b_{j-l}\,b_{l-k}\,b_k\,. \tag{44b}$$

The above recursion relations can be solved explicitly for the coefficients of the Laurent series. In order to verify that there is an arbitrary coefficient at each of the resonances $j=r$, we solve a number of matrix equations of the form

$$\begin{pmatrix} A_{11}(a_{j-1},b_{j-1}) & A_{12}(a_{j-1},b_{j-1}) \\ A_{21}(a_{j-1},b_{j-1}) & A_{22}(a_{j-1},b_{j-1}) \end{pmatrix}\begin{pmatrix} a_j \\ b_j \end{pmatrix}=\begin{pmatrix} B_1(a_{j-1},b_{j-1}) \\ B_2(a_{j-1},b_{j-1}) \end{pmatrix}$$

and find additional constraints on the parameters in order for the determinant of the matrix **A** to vanish at the resonances $j=r$. We then have to check that these constraints are also satisfied by the full matrix equation at the resonance. If there is an arbitrary coefficient at each resonance, then the system is P-type for the corresponding parameters. The algebraic symbol manipulation package REDUCE facilitated the algebra at this step. The P-type cases are listed below:

Case 1(i)

(I) $$C=0,\quad D=0,\quad G=F=E, \tag{45}$$

(II) $$D=-C/3,\quad G=F=E=2C^2/9B\,. \tag{46}$$

Case 1(ii)

(III) $$B=A,\quad D=C=0,\quad G=F/3=E, \tag{47}$$

(IV) $$B=A,\quad D=-C,\quad G=F/3=E\,. \tag{48}$$

Case 2(ii)

(V) $$B=A/4,\quad D=C=0,\quad G=F/6=E/16, \tag{49}$$

(VI) $$B=A/4,\quad D=C=0,\quad G=F/3=E/8\,. \tag{50}$$

Case 3(ii)

(VII) $$B=4A+4D^2/3E,\quad D=-C/8,\quad G=8F/3=8E, \tag{51}$$

(VIII) $$B=4A-6D^2/3E-DC/3E,\quad G=8F/3=16E\,. \tag{52}$$

Thus we find that the generalised Hamiltonian considered here, equation (14), exhibits only four P-type cases (II, IV, VII, VIII) in addition to those special cases (I, III, V, VI) reported earlier by Lakshmanan and Sahadevan (1985) for the reduced Hamiltonian with no cubic terms ($C=D=0$).

4. Additional Conserved Quantities

A Hamiltonian system with N degrees of freedom is integrable if and only if there exist N independent isolating integrals that are in involution (a set of functions is in involution if the Poisson bracket for all pairs vanishes).

In the case of the two-dimensional Hamiltonian we have been studying it is sufficient to explicitly establish the existence of just one additional constant of the motion.

For each of the P-type cases identified above, equations (45)–(52), we have conducted a systematic search for invariants which are polynomial up to order four in the velocities. The most general form for such invariants is (Hietarinta 1983, 1987; Lakshmanan and Sahadevan 1985):

$$I = z_1 \dot{x}^4 + z_2 \dot{x}^3 \dot{y} + z_3 \dot{x}^2 \dot{y}^2 + z_4 \dot{x}\dot{y}^3 + z_5 \dot{y}^4 + z_6 \dot{x}^2 + z_7 \dot{x}\dot{y} + z_8 \dot{y}^2 + z_9 , \tag{53}$$

where the z_i are functions of (x, y) alone. It may be that invariants if they exist are of higher order than four in the velocities or are not simple polynomials in the velocities. The method for searching for integrals of the form (53), whose Poisson bracket

$$\{I, H\} = \frac{\partial I}{\partial \dot{x}} \ddot{x} + \frac{\partial I}{\partial \dot{y}} \ddot{y} + \frac{\partial I}{\partial x} \dot{x} + \frac{\partial I}{\partial y} \dot{y} \tag{54}$$

vanishes, is described in Lakshmanan and Sahadevan (1985). Using this method we established that all P-type cases identified above have non-trivial invariants (i.e. those that are functionally independent of the Hamiltonian) expressible in the form (53). The P-type cases and the non-trivial invariants obtained from this analysis are listed below. The cases with $C = D = 0$, which have been derived previously by Lakshmanan and Sahadevan (1985), are also listed here for completeness:

(I) $$C = 0, \quad D = 0, \quad G = F = E,$$
$$I = (A - B)[Ex^4 + Ex^2y^2 + 2Ax^2 + 2\dot{x}^2] - E[x\dot{y} - y\dot{x}]^2 . \tag{55}$$

(II) $$D = -C/3, \quad G = F = E = 2C^2/9B,$$
$$\begin{aligned} I \;=\; & 4C^2[x\dot{y} - y\dot{x}]^2 + 4AC^2y^2[y^2 + x^2] - 12ABCy[x^2 + 2y^2] + 9AB^2[x^2 + 4y^2] \\ & + 12BC\dot{x}[x\dot{y} - y\dot{x}] + 9B[\dot{x}^2 + 4A\dot{y}^2] . \end{aligned} \tag{56}$$

(III) $$B = A, \quad D = C = 0, \quad G = F/3 = E,$$
$$I = Exy[x^2 + y^2] + Axy + \dot{x}\dot{y} . \tag{57}$$

(IV) $$B = A, \quad D = -C, \quad G = F/3 = E,$$
$$I = 3Exy[x^2 + y^2] + 3Axy + 3\dot{x}\dot{y} - Cx[x^2 + 3y^2] . \tag{58}$$

(V) $$B = A/4, \quad D = C = 0, \quad G = F/6 = E/16,$$
$$I = Exy^2[2x^2 + y^2] + 4Axy^2 + 16\dot{y}[y\dot{x} - x\dot{y}] . \tag{59}$$

(VI) $$B = A/4, \quad D = C = 0, \quad G = F/3 = E/8,$$
$$\begin{aligned} I \;=\; & E^2[2x^2y^2 + y^4]^2 + 8AEy^4[2x^2 + y^2] + 32E[y^4(\dot{x}^2 + \dot{y}^2) \\ & + 2xy^2\dot{y}(3x\dot{y} - 2y\dot{x})] + [4Ay^2 + 16\dot{y}^2]^2 . \end{aligned} \tag{60}$$

(VII)
$$B=4A+4D^2/3E, \quad D=-C/8, \quad G=8F/3=8E,$$
$$\begin{aligned} I = {} & 81E^5[x^4+2x^2y^2]^2+216DE^4x^4y[x^2+2y^2]+324AE^4[x^2+2y^2] \\ & +324E^4x^2[x^2(\dot{x}^2+\dot{y}^2)-2\dot{x}y(2x\dot{y}-3y\dot{x})]+324E^3[Ax^2+\dot{x}^2]^2 \\ & +432DE^3x^2\dot{x}[3y\dot{x}-x\dot{y}]+432ADE^3x^2y[3x^2+4y^2]-72D^2E^3x^6 \\ & -192E^2D^3x^2y[x^2+y^2]+144AD^2E^2x^2[x^2+12y^2]+1728DA^2E^2x^2y \\ & +192ED(9AE-D^2)\dot{x}[x\dot{y}-y\dot{x}]-16ED^4x^2[x^2+12y^2]-192AED^4x^2y \\ & -64D^2(9AE-D^2)[Ax^2+\dot{x}^2]. \end{aligned} \tag{61}$$

(VIII)
$$B=4A-6D^2/3E-DC/3E, \quad G=8F/3=16E,$$
$$\begin{aligned} I = {} & 24E^2x^2y[x^2+2y^2]+12EDx^2[x^2+2y^2]+CEx^4+24AEx^2y \\ & +2A(6D+C)x^2+2(6D+C)\dot{x}^2+24E\dot{x}[x\dot{y}-y\dot{x}]. \end{aligned} \tag{62}$$

Thus, we have verified that each of the P-type cases listed in Section 3 is integrable by explicitly deriving additional constants of the motion for each case.

5. Discussion

Consider the following two physical cases of interest:

(i) $B=3A$, $D=C/3$, $G=3F=9E$. This corresponds to the four-particle chain with end particles held fixed and with linear ($A\neq 0$), quadratic ($C\neq 0$), and cubic ($E\neq 0$) interparticle forces, equation (12). Our analysis shows that if we restrict $E\neq 0$, $F\neq 0$, $G\neq 0$ then the system is not P-type in this case for any values of the parameters. Note, however, that the four-particle chain with the ends held fixed, and with linear and cubic interparticle forces ($B=3A$, $D=C=0$, $G=3F=9E$) is 'close' to the integrable case VII. The additional conserved quantity in case VII, equation (61) may be 'approximately' conserved in this physical system.

(ii) $B=A$, $D=C$, $G=F=E$. This corresponds to the three-particle periodic chain with linear ($A\neq 0$), quadratic ($C\neq 0$), and cubic ($E\neq 0$) interparticle forces, equation (13). Our analysis shows that if we restrict $E\neq 0$, $F\neq 0$, $G\neq 0$ then the system can only be P-type in this case if $D=C=0$. Physically these parameter values correspond to the three-particle periodic chain with linear and cubic interparticle forces. In terms of the particle coordinates, the invariant in this case is given by

$$I \propto x_1(\dot{x}_3-\dot{x}_2)+x_2(\dot{x}_1-\dot{x}_3)+x_3(\dot{x}_2-\dot{x}_1).$$

Note that the three-particle periodic chain with linear and quadratic interparticle forces ($B=A$, $D=C$, $G=F=E=0$) is equivalent to the Henon–Heiles (1964) Hamiltonian (Lunsford and Ford 1972)—a paradigm model for non-integrability (Bountis *et al.* 1982; Chang *et al.* 1982) and chaos (Ford 1975) in a two degrees of freedom system.

Our analysis has also shown that of the four non Z-type cases found by Yoshida *et al.* (1988) for the Hamiltonian (14) with $B = A$, $G = F = E$, only two are P-type: $D = C = 0$; $D = -C/3$, $E = 2C^2/9A$. We established the integrability of the two non Z-type, P-type cases by constructing non-trivial invariants that are polynomial up to order four in the velocities (equations 55 and 56). We have also conducted a systematic search for invariants which are polynomial up to order 4 in the velocities for the two non Z-type, non P-type cases: $D = -C/2$; $D = C$, $E = 2C^2/9A$. This search ruled out the possibility of any non-trivial invariants of the form (53). Thus, the analysis here strongly suggests that whilst these cases are non Z-type they are also not integrable.

The analysis above demonstrates the sensitivity of integrability properties (and therefore energy sharing) to the types of boundary conditions and the particular form of interatomic potential. Integrability properties are also sensitive to the number of degrees of freedom in the system (see e.g. the review by Ramani *et al.* 1989). To date there have been few algebraic results reported for systems with many degrees of freedom. Lakshmanan and Sahadevan (1985) have carried out a Painlevé analysis for a system of N coupled quartic anharmonic oscillators. Yoshida (1989) has established sufficient conditions for non-integrability for N degrees of freedom Hamiltonian systems with a homogeneous potential.

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References

Ablowitz, M. J., Ramani, A., and Segur, H. (1980). *J. Math. Phys.* **21**, 715.
Ashcroft, N. W., and Mermin, N. D. (1976). 'Solid State Physics', p. 427 (Saunders College: Philadelphia).
Bountis, T., Segur, H., and Vivaldi, F. (1982). *Phys. Rev.* A **25**, 1257.
Chang, Y. F., Tabor, M., and Weiss, J. (1982). *J. Math. Phys.* **23**, 531.
Ford, J. (1975). *In* 'Fundamental Problems in Statistical Mechanics', Vol. 3 (Ed. E. D. G. Cohen), p. 215 (North-Holland: Amsterdam).
Henon, M., and Heiles, C. (1964). *Astron. J.* **69**, 73.
Hietarinta, J. (1983). *Phys. Lett.* A **96**, 273.
Hietarinta, J. (1987). *Phys. Rep.* **147**, 87.
Lakshmanan, M., and Sahadevan, R. (1985). *Phys. Rev.* A **31**, 861.
Lunsford, G. H., and Ford, J. (1972). *J. Math. Phys.* **13**, 700.
Ramani, A., Dorizzi, B., and Grammaticos, B. (1982). *Phys. Rev. Lett.* **49**, 1539.
Ramani, A., Grammaticos, B., and Bountis, T. (1989). *Phys. Rep.* **180**, 159.
Steeb, W.-H., Klobe, M., Spieker, B. M., and Kunick, A. (1985). *Found. Phys.* **15**, 637.
Toda, M. (1981). 'Theory of Nonlinear Lattices' (Springer: Berlin).
Yoshida, H. (1989). *In* 'Singular Behaviour and Nonlinear Dynamics' (Eds St. Pnevmatikos *et al.*), p. 114 (World Scientific: Singapore).
Yoshida, H., Grammaticos, B., and Ramani, A. (1987). *Acta Appl. Math.* **8**, 75.
Yoshida, H., Ramani, A., and Grammaticos, B. (1988). *Physica* D **30**, 151.

Appendix: Table of Identities

$$\sum_{n=1}^{N} \sin\left(\frac{n\pi s}{N+1}\right) \sin\left(\frac{n\pi s'}{N+1}\right) = \frac{N+1}{2}\,\delta_{s,s'}\,, \tag{A1}$$

$$\sum_{n=0}^{N} \exp\,[\mathrm{i}\,\pi r(n+\tfrac{1}{2})/(N+1)] =$$
$$\begin{cases} +(N+1) & r = 2q(N+1) \quad q = 0, \pm 2, \pm 4, \ldots, \\ -(N+1) & r = 2q(N+1) \quad q = \pm 1, \pm 3, \ldots, \\ \frac{\mathrm{i}}{\omega_r}[1 - \exp\,(\mathrm{i}\,\pi r)] & r \neq 2q(N+1) \quad \omega_r = 2\sin\left(\frac{r\pi}{2(N+1)}\right), \end{cases} \tag{A2}$$

$$\sum_{n=1}^{N} \exp[\mathrm{i}\,2\pi rn/N] = \begin{cases} +N & r = qN \quad q = 0, \pm 1, \pm 2, \ldots, \\ 0 & r \neq qN, \end{cases} \tag{A3}$$

$$\sum_{n=1}^{N} \exp[\mathrm{i}\,2\pi r(n-\tfrac{1}{2})/N] = \begin{cases} +N & r = qN \quad q = 0, \pm 2, \pm 4, \ldots, \\ -N & r = qN \quad q = \pm 1, \pm 3, \ldots, \\ 0 & r \neq qN. \end{cases} \tag{A4}$$

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