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Integrability of the Toda chain with free boundaries

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Abstract. The Hamilton function for the Toda chain with free boundaries is studied for different interaction and mass parameters. For certain systems the connection to simple Lie algebras is shown and the integrability is proved by constructing the corresponding Lax representations. For the four-particle system a Painlevé analysis is presented.

1. Introduction

In recent years the question of whether a given many-particle system is integrable or not has been studied intensively for various models. Although there exists no general method for an integrability test of a Hamiltonian system, there are some mathematical constructive methods for integrable systems (Ablowitz *et al* 1978, 1980, Bogoyavlensky 1976, Bountis *et al* 1982, Dorizzi *et al* 1983, 1984, Grammaticos *et al* 1983, Olshanetsky and Perelomov 1981, Ramani *et al* 1982). In the following a one-dimensional discrete chain with exponential interaction (Toda lattice) is studied in some detail for free boundary conditions. The system has been investigated by Bogoyavlensky (1976) for periodic boundary conditions, and for equal masses it was shown by Moser (1975) that the lattice is integrable even for free boundaries. By integrability of a system of N degrees of freedom the existence of N analytic global integrals of motion which are in involution is implied (e.g. Thirring 1978). In this paper it will be proven by using group theoretical methods that for certain parameters the open end Toda chain is integrable. For the corresponding four-particle system we have verified that the method of the Painlevé property (Ablowitz *et al* 1978, 1980) leads to the same integrability parameters.

The Toda chain with alternating masses is known to be non-integrable and it was shown quite recently that its mixing behaviour in phase space may support the transfer of heat according to the Fourier law (Mokross and Büttner 1983). It is therefore interesting to know open end systems which are integrable in order to study the transition to non-integrability for such fundamental problems as the heat conduction.

In § 2 the results for the general N-particle chain are presented. In § 3 certain scaling properties are discussed. In the appendix two special cases for a four- and five-particle system are treated by a Painlevé analysis and algebraic methods, respectively.

2. The open end Toda chain

In the following the Hamiltonian for N particles with free end boundary conditions is studied in detail. As parameters we have the different masses m_i at each lattice site

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i and the strength of the exponential interaction ε_i between neighbouring sites. With the displacement q_i and the corresponding momentum p_i the Hamiltonian is written as

$$H=\sum_{i=1}^{N-1}\{p_i^2/2m_i+\exp[\varepsilon_i(q_i-q_{i+1})]/\varepsilon_i\}+p_N^2/2m_N. \tag{1}$$

For the following investigations it is useful to introduce the centre of mass coordinates as well as the relative displacements by a canonical transformation:

$$q'_N=\sum_{i=1}^{N} m_iq_i \qquad p'_N=\sum_{i=1}^{N} p_i/M_N \qquad M_i=\sum_{j=1}^{i} m_j \tag{2}$$

$$q'_i=\varepsilon_i(q_i-q_{i+1}) \qquad p'_i=\left(\sum_{l=1}^{i} p_l-M_ip'_N\right)\varepsilon_i^{-1} \qquad i=1,\ldots,N-1. \tag{3}$$

In these variables the function H is transformed into

$$H=M_Np_N'^2/2+\sum_{i=1}^{N-1}\varepsilon_i^2(m_i+m_{i+1})p_i'^2/(2m_im_{i+1})$$
$$-\sum_{i=1}^{N-2}\varepsilon_i\varepsilon_{i+1}p'_ip'_{i+1}/m_{i+1}+\sum_{i=1}^{N-1}\exp(q'_i)/\varepsilon_i. \tag{4}$$

In a second step a scaling transformation is introduced:

$$t''=\alpha^{-1/2}t \qquad p''_i=\alpha^{-1/2}p'_i \qquad q''_i=q'_i-\ln\varepsilon_i \tag{5}$$

with $\alpha=m_2/\varepsilon_1\varepsilon_2$. By this special scaling the masses m_1 and m_2 are used as reference, but other choices are possible. The Hamiltonian is transformed to (neglecting the centre of mass motion)

$$H=\sum_{i=1}^{N-1}\alpha\varepsilon_i^2(m_i+m_{i+1})p_i''^2/(2m_im_{i+1})-\sum_{i=1}^{N-2}\alpha\varepsilon_i\varepsilon_{i+1}p''_ip''_{i+1}/m_{i+1}+\sum_{i=1}^{N-1}\exp q''_i. \tag{6}$$

This Hamiltonian is now in a form which allows the application of theorem 1 from Bogoyavlensky (1976). From this theorem it follows that Hamiltonians of the form

$$H=\sum_{i=1}^{N-1}[p_i''^2+\exp(q''_i)]-\sum_{i=2}^{N-1}p''_{i-1}p''_i+\begin{cases}0 & \text{case 1}\\ -p''^2_{N-1}/2 & \text{case 2}\\ +p''^2_{N-1}-p''_{N-2}p''_{N-1} & \text{case 3}\end{cases} \tag{7}$$

are integrable, because they can be deduced from the Lie algebras A_{N-1}, B_{N-1}, C_{N-1} in case 1, 2 and 3, respectively. Note that the matrices M with elements $m_{ij}=2a_{ij}/a_{ii}$, where a_{ij} is the coefficient of the momentum term $p''_ip''_j$ in (7), are just the Cartan matrices for A_{N-1}, B_{N-1}, C_{N-1} (e.g. Humphreys 1972). By comparison of (6) and (7) we arrive at the integrability conditions for the mass and coupling parameters.

Case 1:

$$\varepsilon_i^2(m_i+m_{i+1})m_2=2m_im_{i+1}\varepsilon_1\varepsilon_2 \qquad i=1,\ldots,N-1$$
$$\varepsilon_i\varepsilon_{i-1}m_2=m_i\varepsilon_1\varepsilon_2 \qquad i=2,\ldots,N-1. \tag{8}$$

Case 2:
For $i=N-1$ the above condition is changed:

$$\varepsilon_{N-1}^2(m_{N-1}+m_N)m_2=m_{N-1}m_N\varepsilon_1\varepsilon_2 \qquad \varepsilon_{N-2}\varepsilon_{N-1}m_2=m_{N-1}\varepsilon_1\varepsilon_2. \tag{9}$$

Case 3:
Again for $i=N-1$ a change is necessary:

$$\varepsilon_{N-1}^2(m_{N-1}+m_N)m_2=4m_{N-1}m_N\varepsilon_1\varepsilon_2 \qquad \varepsilon_{N-2}\varepsilon_{N-1}m_2=2m_{N-1}\varepsilon_1\varepsilon_2. \tag{10}$$

It is obvious that the different cases are distinct mainly due to the boundary term for the Nth particle and the $(N-1)$th interaction.

By scaling this condition to the case $m_1=\varepsilon_1=1$ which is always possible for a certain length and energy scale these relations can be reduced to the following conditions.

Case 1:

$$\begin{aligned} m_i &= 2m_2(1+m_2)/[i-1-(i-3)m_2]/[i-(i-2)m_2] \qquad && i=1,\ldots,N \\ \varepsilon_i &= (1+m_2)/[i-(i-2)m_2] && i=2,\ldots,N-1. \end{aligned} \tag{11}$$

Since the mass parameters have to be positive, the value of m_2 has to be in the interval: $m_2\in(0, 1+2/(N-2))$.

Case 2:
There is only a change in the boundary term

$$\begin{aligned} m_N &= 2m_2(1+m_2)/\{(1-m_2)[N-1-(N-3)m_2]\} \\ \varepsilon_{N-1} &= (1+m_2)/[N-1-(N-3)m_2] \end{aligned} \tag{12}$$

and $m_2\in(0,1)$.

Case 3:

$$\begin{aligned} m_N &= 2m_2(1+m_2)/\{(1-m_2)[N-1-(N-3)m_2]\} \\ \varepsilon_{N-1} &= 2(1+m_2)/[N-1-(N-3)m_2] \end{aligned} \tag{13}$$

and $m_2\in(0,1)$.

In order to find the explicit representation of the equations of motion in the so-called Lax form (with matrices L, B)

$$\mathrm{d}L/\mathrm{d}t=LB-BL \tag{14}$$

we can apply the general method exposed by Bogoyavlensky (1976) together with the well known matrix representations of the Lie algebras A_N, B_N, C_N (e.g. Gilmore 1974). The matrices L and B for case 1 are already known (Moser 1975). Setting $l_i=\exp(q_i'')/2$ for $i=1,\ldots,N-1$ and by scaling the momenta p_i'' and the time t'' by a factor $\sqrt{2}$ the matrices L and B for case 2 are given by

$$L=\begin{bmatrix} L_1 & L_2 \\ L_3 & L_4 \end{bmatrix} \qquad B=\begin{bmatrix} B_1 & B_2 \\ B_3 & B_4 \end{bmatrix} \tag{15}$$

where L_1 is the $N\times N$ matrix

$$L_1=\begin{bmatrix} p_1 & l_1/2 & 0 \ldots\ldots & & & & \\ l_1 & p_2-p_1 & l_2/2 & 0\ldots\ldots & & & \\ 0 & l_2 & p_3-p_2 & l_3/2 & 0\ldots\ldots & & \\ & & \ldots\ldots & & l_{N-2} & p_{N-1}-p_{N-2} & l_{N-1}/2 \\ & & \ldots\ldots & & & l_{N-1} & 0 \end{bmatrix} \tag{16}$$

and L_4 is the $(N-1)\times(N-1)$ matrix

$$L_4=\begin{bmatrix} p_{N-2}-p_{N-1} & -l_{N-2}/2 & 0\ldots\ldots\ldots\ldots & & & \\ -l_{N-2} & p_{N-3}-p_{N-2} & -l_{N-3}/2 & 0\ldots\ldots & & \\ & & \ldots\ldots\ldots\ldots\ldots & -l_2 & p_1-p_2 & -l_1/2 \\ & & \ldots\ldots\ldots\ldots\ldots\ldots & & -l_1 & -p_1 \end{bmatrix}. \tag{17}$$

In addition L_2 is an $N\times(N-1)$ matrix with

$$(L_2)_{ij}=-l_{N-1}\delta_{i,N}\delta_{j,1}/2 \tag{18}$$

and L_3 an $(N-1)\times N$ matrix with

$$(L_3)_{ij}=-l_{N-1}\delta_{i,1}\delta_{j,N}. \tag{19}$$

The corresponding matrix B has the submatrices $B_2=L_2$ and $B_3=-L_3$. The matrices B_1 and B_4 are constructed from L_1 and L_4 by neglecting the diagonal elements and changing the sign of the subdiagonal elements. The $(N-1)$ constants of motion I_k are then implicitly given by

$$I_k=\mathrm{Tr}(L^{2k}) \qquad \text{for } k=1,\ldots,N-1. \tag{20}$$

They follow from the theory of polynomial invariants (Chevalley 1955). For case 3 it is possible to construct similar matrices

$$L=\begin{bmatrix} L_1 & L_2 \\ L_2^t & -\tilde{L}_1 \end{bmatrix} \qquad B=\begin{bmatrix} B_1 & B_2 \\ -B_2^t & -\tilde{B}_1 \end{bmatrix} \tag{21}$$

where L_1 can be written in the form

$$L_1=\begin{bmatrix} p_1 & l_1/2\ldots\ldots\ldots\ldots\ldots\ldots & & & \\ l_1 & p_2-p_1 & l_2/2\ldots\ldots\ldots\ldots & & \\ & \ldots\ldots\ldots\ldots l_{N-3} & p_{N-2}-p_{N-3} & l_{N-2}/2 \\ & \ldots\ldots\ldots\ldots\ldots\ldots & l_{N-2} & 2p_{N-1}-p_{N-2} \end{bmatrix}. \tag{22}$$

$\tilde{L}_1$ is related to L_1 by a reflection at the minor diagonal of L. Here the matrix L_2 has here the dimension $(N-1)\times(N-1)$ and is defined by

$$(L_2)_{ij}=l_{N-1}\,\delta_{i,N-1}\,\delta_{1,j}. \tag{23}$$

L_2^t is the transpose of L_2. The corresponding submatrices B_1 and B_4 are constructed as in case 2. Furthermore, we have $L_2=B_2$ and the constants of motion are constructed in the same way as above (20).

Besides the general results for N-particle systems there may be additional integrable cases for certain finite numbers of particles that are related to exceptional Lie algebras. As an example we discuss in appendix 2 the five-particle system related to the algebra F_4.

3. Scaling properties

For a special choice of parameters, the Hamiltonian for case 1 is identical to that of a chain with equal masses and equal interaction parameters. One arrives at $m_i=\varepsilon_i=1$

for $m_1 = \varepsilon_1 = 1$ and $m_2 = 1$:

$$H = \sum_{i=1}^{N} p_i^2/2 + \sum_{i=1}^{N-1} \exp(q_i - q_{i+1}). \tag{24}$$

One can show that the general Hamiltonian (1) can be transformed to (24) if the parameters m_i and ε_i are chosen according to the integrability condition (8). The transformation is most readily defined in the variables

$$b_i = -p_i/2m_i \qquad a_i = \tfrac{1}{2}\exp[-\varepsilon_i(q_{i+1} - q_i)/2] \tag{25}$$

and is

$$\begin{aligned} b'_1 &= \beta_{1,1} b_1 = \varepsilon_1(m_1 + m_2) b_1/2m_2 \\ a'_1 &= (\beta_{1,1}/m_1)^{1/2} a_1 \\ b'_i &= \sum_{j=1}^{i} \beta_{i,j} b_{i+1-j} \\ a'_i &= \alpha_i a_i \end{aligned} \tag{26}$$

where we have used

$$\begin{aligned} &\beta_{i,1} = \varepsilon_{i-1} \qquad \alpha_i^2 = \varepsilon_{i-1}/m_i && \text{for } i > 2 \\ &\beta_{i,2} = \beta_{i-1,1} - \varepsilon_{i-1} && \text{for } i > 2 \\ &\beta_{i,k} = \beta_{i-1,k-1} && \text{for } k > 3,\ i > 3. \end{aligned} \tag{27}$$

The corresponding momenta and displacements are subject to the same equations of motion as those resulting from (24).

A similar transformation can be made for case 2 if one chooses $m_1 = \varepsilon_1 = 1$, $m_2 = \frac{1}{3}$. Then we have

$$m_i = 2/i(i+1) \qquad \varepsilon_{i-1} = 2/i \qquad m_N = 2/N \tag{28}$$

and each system which is integrable under case 2 can be transformed to this special case. We do not give here the details of the scaling transformation because they are quite similar to those discussed for case 1, but note that this special choice of masses and interaction constants does not seem to be very physical since these parameters are site-dependent and decrease with increasing length of the chain. But for smaller systems like, for example, a four-particle Toda molecule (with open ends) case 2 and case 3 represent interesting integrable systems where one can study the transition to non-integrability. The results for $N = 3$ are related to those of Bountis *et al* (1982), although there is an additional integrable case resulting from the algebra G_2. For the four-particle system it can be shown that an analysis of the Painlevé properties results in the same integrability conditions as found above (see appendix 1).

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Appendix 1. Painlevé analysis for the four-particle system

In this appendix we represent a Painlevé analysis for the general four-particle system with exponential interaction and free boundaries. It shows that the algebraic methods discussed above support the analytic investigations at least for small numbers of particles. The general Hamiltonian is scaled to the form

$$H = p_1^2/2 + p_2^2/2m_2 + p_3^2/2m_3 + p_4^2/2m_4 + \exp(q_1 - q_2) + \exp[-\varepsilon_1(q_3 - q_2)]/\varepsilon_1 + \exp[-\varepsilon_2(q_4 - q_3)]/\varepsilon_2. \tag{A1.1}$$

Introducing new variables

$$b_1 = -p_1/2 \qquad b_2 = -p_2/2m_2 \qquad b_3 = -p_3/2m_3 \qquad b_4 = -p_4/2m_4$$
$$a_1 = \tfrac{1}{2}\exp[-(q_2 - q_1)/2] \qquad a_2 = \tfrac{1}{2}\exp[-\varepsilon_1(q_3 - q_2)/2] \tag{A1.2}$$
$$a_3 = \tfrac{1}{2}\exp[-\varepsilon_2(q_4 - q_3)/2]$$

one finds the equations of motion (neglecting centre of mass motion):

$$\dot a_1 = a_1(b_2 - b_1) \qquad \dot b_1 = 2a_1^2 \tag{A1.3}$$
$$\dot a_2 = -\varepsilon_1 a_2[b_1 + (m_2 + m_3)/b_2 + m_4 b_4]m_3^{-1} \qquad \dot b_2 = 2(a_2^2 - a_1^2)/m_2 \tag{A1.4}$$
$$\dot a_3 = \varepsilon_2 a_3[b_1 + m_2 b_2 + (m_3 + m_4)b_4]/m_3 \qquad \dot b_4 = -2a_3^2/m_4. \tag{A1.5}$$

Using the algorithm proposed by Ablowitz *et al* (1980) one has for the behaviour in the vicinity of a pole at $t = t_0$

$$a_1 \sim \alpha_1 \tau^x \qquad a_2 \sim \alpha_2 \tau^y \qquad a_3 \sim \alpha_3 \tau^z \tag{A1.6}$$

with $\tau = t - t_0$.

From the equations for b_1 and b_4 one finds

$$b_1 \sim \tau^{2x+1} \qquad b_4 \sim \tau^{2z+1} \tag{A1.7}$$

and three different cases for b_2:

$$\begin{aligned} &\text{(i)} && y = x && b_2 \sim \tau^{2x+1} \\ &\text{(ii)} && y > x && b_2 \sim \tau^{2x+1} \\ &\text{(iii)} && y < x && b_2 \sim \tau^{2y+1}. \end{aligned} \tag{A1.8}$$

Each of these splits in two different special cases:

$$\begin{aligned} &\text{(i}a\text{)} && x = y = z = -1 && \text{(i}b\text{)} && x = y = -1 \text{ and } z > -1 \\ &\text{(ii}a\text{)} && x = z = -1 \text{ and } y > -1 && \text{(ii}b\text{)} && x = -1 \text{ and } y, z > -1 \\ &\text{(iii}a\text{)} && y = z = -1 \text{ and } x > -1 && \text{(iii}b\text{)} && y = -1 \text{ and } x, z > -1. \end{aligned} \tag{A1.9}$$

A comparison of the coefficient for the leading terms yields relations between the exponents x, y, z and the parameters m_2, m_3, m_4 and ε_1, ε_2. Since the exponents have to be integers or half-integers (Bountis *et al* 1982) and also the exponents of the resonances, one finds, after some tedious calculations, five integrability regions with

Painlevé properties. Two of these are equivalent, which can be seen by a rescaling transformation. The others are identical to those found by the algebraic analysis:

$$(a)\quad m_3=\frac{m_2(1+m_2)}{3-m_2}\qquad m_4=\frac{m_3}{2-m_2}\qquad \varepsilon_1=\frac{1+m_2}{2}\qquad \varepsilon_2=\frac{1+m_2}{3-m_2} \tag{A1.10}$$

$$(b)\quad m_3,\ \varepsilon_1 \text{ as above}\qquad m_4=\frac{2m_3}{1-m_2}\qquad \varepsilon_2=\frac{1+m_2}{3-m_2} \tag{A1.11}$$

$$(c)\quad m_3,\ \varepsilon_1 \text{ as above}\qquad m_4=\frac{2m_3}{1-m_2}\qquad \varepsilon_2=\frac{2(1+m_2)}{3-m_2}. \tag{A1.12}$$

Appendix 2. Example of an exceptional Lie algebra

The general results discussed above can be extended for a certain number of particles by the use of exceptional Lie algebras. As an example we discuss the relation between F_4 and a five-particle system (with fixed centre of mass). From the Cartan matrix for F_4 one can conclude that the Hamiltonian

$$H=p_1^2+p_2^2+2p_3^2+2p_4^2-p_1p_2-2p_2p_3-2p_3p_4 \\ +\exp(q_1)+\exp(q_2)+\exp(q_3)+\exp(q_4) \tag{A2.1}$$

describes an integrable system. A comparison with our general transformed Hamiltonian yields the integrability conditions:

$$\begin{array}{lll} \varepsilon_1^2\alpha/\mu_{1,2}=2 & \varepsilon_2^2\alpha/\mu_{2,3}=2 & \varepsilon_3^2\alpha/\mu_{3,4}=4 \\ \varepsilon_4^2\alpha/\mu_{4,5}=4 & \varepsilon_2\varepsilon_3\alpha=2m_3 & \varepsilon_3\varepsilon_4\alpha=2m_4 \end{array} \tag{A2.2}$$

with the reduced masses $1/\mu_{ij}=1/m_i+1/m_j$. For the choice $\varepsilon_1=m_1=1$ this results in

$$\begin{array}{lll} m_3=\dfrac{m_2(1+m_2)}{3-m_2} & m_4=2\dfrac{m_3}{1-m_2} & m_5=\dfrac{2m_2(1+m_2)}{(1-3m_2)(1-m_2)} \\ \varepsilon_2=(1+m_2)/2 & \varepsilon_3=2(1+m_2)/(3-m_2) & \varepsilon_4=(1+m_2)/(1-m_2) \end{array} \tag{A2.3}$$

with $m_2\in(0,\frac{1}{3})$.

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