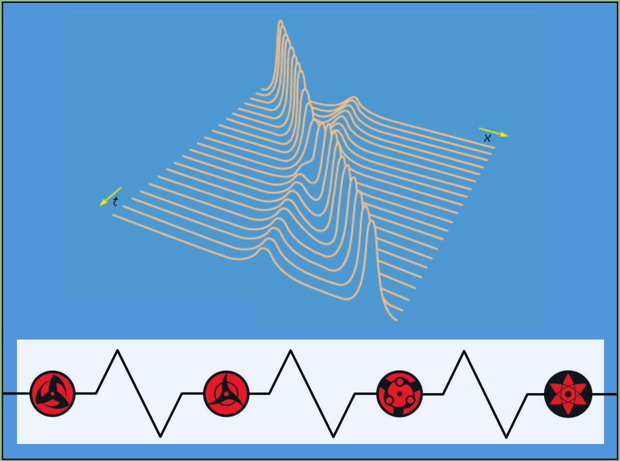

1D Toda Lattices

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What are crystals?

A solid material whose constituents (such as atoms, molecules, or ions) are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions.

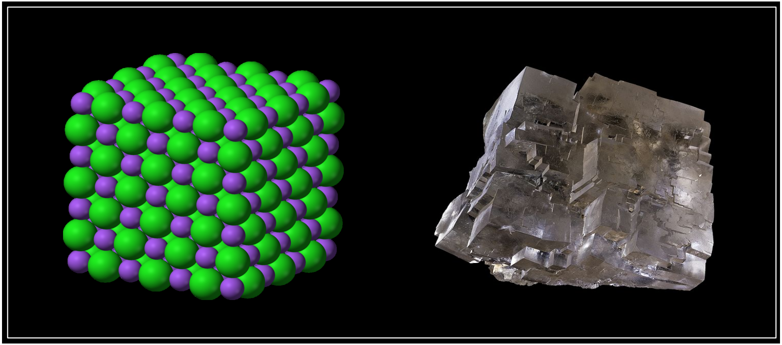
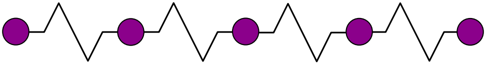


Figure: Halite (table salt, NaCl)

1 dimensional crystals

In a crystal, electrons move in a potential, produced by regularly spaced ion cores.



Assumptions:

Particles have unit mass

Finitely many particles

Terminology:

Open : no boundary conditions

Closed : periodic boundary condition or particles on a ring

Method:

Hamilton's formalism

What is a Hamiltonian?

A Hamiltonian system is a dynamical system governed by Hamilton's equations. Examples include planetary system and electron in an electromagnetic field.

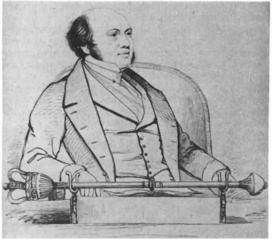


Figure: Sir William Rowan Hamilton (1805-1865)

It is a mathematical formalism developed by Hamilton to describe the evolution equations of a physical system.

Let the phase space be $\mathbb{R}^k$ and consider a system of n particles. The Hamiltonian $H = H(\mathbf{p}, \mathbf{q}, t)$ is a scalar function, where $\mathbf{p}$ and $\mathbf{q}$ denote the momentum and position of n particles. Thus, $\mathbf{p} = (p_1, \ldots, p_n)$ and $\mathbf{q} = (q_1, \ldots, q_n)$, vectors in $\mathbb{R}^{kn}$, are functions of time t.

Hamilton's evolution equations:

$$\begin{aligned} \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{q}} \\ \frac{d\mathbf{q}}{dt} &= \frac{\partial H}{\partial \mathbf{p}} \end{aligned}$$

If the Hamiltonian is not time dependent, then it becomes conserved throughout the motion. Springs, pendulum are examples where H, a constant of motion, equals the energy E of the system.

Harmonic Oscillator

Consider $\mathbf{p} = p$ and $\mathbf{q} = x$ with $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$. Evolution equations are

$$\frac{dp}{dt} = -kx, \quad \frac{dx}{dt} = \frac{p}{m}.$$

In matrix form, we have

$$\begin{pmatrix} p'(t) \\ x'(t) \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & -k \\ \frac{1}{m} & 0 \end{pmatrix}}_{A} \begin{pmatrix} p(t) \\ x(t) \end{pmatrix}$$

From ordinary differential equations, we know that $(c = k/m)$

$$\begin{pmatrix} p(t) \\ x(t) \end{pmatrix} = e^A \begin{pmatrix} p(0) \\ x(0) \end{pmatrix} = \begin{pmatrix} \cos(\sqrt{c}t) & -\sqrt{km}\sin(\sqrt{c}t) \\ \frac{1}{\sqrt{km}}\sin(\sqrt{c}t) & \cos(\sqrt{c}t) \end{pmatrix} \begin{pmatrix} p(0) \\ x(0) \end{pmatrix}$$

History of the Problem

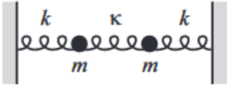
Consider Hamiltonians of the form (for a closed 1D lattice)

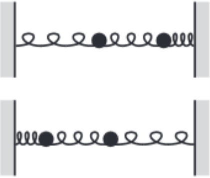
$$H = \sum_{j=1}^{n} \frac{p_j^2}{2} + \sum_{j=1}^{n} V(q_{j+1} - q_j)$$

with *harmonic interaction*, i.e., $V(r) = r^2/2$. Evolution equations are

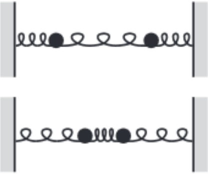
$$\dot{q}_j = p_j, \quad \dot{p}_j = -(2q_j - q_{j-1} - q_{j+1}).$$

This is a system of linear differential equations with constant coefficients. Solution is given by the superposition of normal modes.





Both springs move the same way.
The middle spring is never stretched.
Same amplitude and frequency is $\sqrt{k/m}$.



Both springs move oppositely.
The middle spring exerts a restoring force.
Amplitudes are equal but opposite.
Frequency is $\sqrt{(k+2x)/m}$.

Any arbitrary motion of the system is a linear combination of these two normal modes.

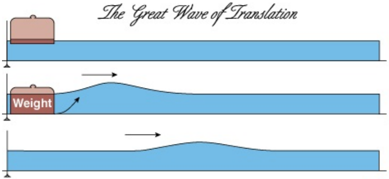
Pictures courtesy David Morin's book (draft) *Waves*.

In 1950's it was believed that a generic non-linear perturbation would lead to thermalization.

1955 Fermi, Pasta, Ulam, Tsingou: Observed a quasi-periodic motion instead of thermalization
1965 Kruskal, Zabusky: Connections to solitons and KdV equation

Solitons arise in a wide variety of disciplines - *non-linear differential equations*, *hydrodynamics*, *non-linear optics (stability)*, *low frequency oscillations in DNA*, *communication engineering*.

A soliton is a solitary wave that maintains its shape while it propogates at constant velocity.



It was first observed in 1834 by naval engineer J. S. Russell.

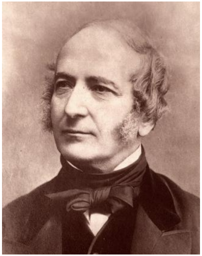


Figure: John Scott Russell (1808-1882)

It was only in 1960's, with the advent of modern computers, that the significance of Scott Russell's observation became apparent. Solitions, by definition, are unaltered in shape and speed by a collision with other solitons. Thus, solitary waves on a water surface are not actually solitons.

1D (Open) Toda Lattice

The search for solition solutions led Morikazu Toda (in 1967) to consider $V(r) = e^{-r} - 1$. It is a simple model for a one dimensional crystal in solid state physics. It is famous because it is one of the earliest examples of a non-linear, completely integrable system.

Popular Interpretation: System of unit masses, connected by non-linear springs subject to exponential restoring force.

$$H(\mathbf{p}, \mathbf{q}, t) = \sum_{i=1}^{n} \frac{p_j^2}{2} + \sum_{j=1}^{n-1} e^{2(q_j - q_{j+1})}$$

Assumptions:

$$p_1 + \cdots + p_n = 0 \qquad \text{(conservation of momentum)}$$
$$q_1 + \cdots + q_n = 0 \qquad \text{(conservation of centre of mass)}$$

Evolution equations are

$$\begin{aligned}
\dot{q}_j &= p_j & j = 1, \ldots, n \\
\dot{p}_1 &= -2e^{2(q_1 - q_2)} & \\
\dot{p}_j &= -2e^{2(q_j - q_{j+1})} + 2e^{2(q_{j-1} - q_j)} & j = 2, \ldots, n-1 \\
\dot{p}_n &= 2e^{2(q_{n-1} - q_n)} &
\end{aligned}$$

Consider the two matrices (with $Q_{i,j} = e^{q_i - q_j}$)

$$L = \begin{pmatrix} p_1 & Q_{1,2} & 0 & \cdots & 0 \\ Q_{1,2} & p_2 & Q_{2,3} & \cdots & 0 \\ 0 & Q_{2,3} & p_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & p_n \end{pmatrix}$$

$$M = \begin{pmatrix} 0 & Q_{1,2} & 0 & \cdots & 0 \\ -Q_{1,2} & 0 & Q_{2,3} & \cdots & 0 \\ 0 & -Q_{2,3} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

We compute $[L,M] := LM = ML$ for $n = 2$. Note that $p_1 + p_2 = 0 = q_1 + q_2$ implies that

$$Q_{1,2} = e^{2q_1} \;\Rightarrow\; \dot{Q}_{1,2} = 2e^{2q_1}\dot{q}_1 = (p_1 - p_2)Q_{1,2}.$$

$$\dot{p}_1 = -2e^{2(q_1-q_2)} = -2e^{4q_1} = -2Q_{1,2}^2$$

$$[L,M] = \begin{pmatrix} -2Q_{1,2}^2 & (p_1 - p_2)Q_{1,2} \\ (p_1 - p_2)Q_{1,2} & 2Q_{1,2}^2 \end{pmatrix} = \begin{pmatrix} \dot{p}_1 & \dot{Q}_{1,2} \\ \dot{Q}_{1,2} & \dot{p}_2 \end{pmatrix} = \dot{L}$$

Theorem

The Lax equation holds, i.e., $\dot{L} = [L, M]$.

Remark Both L and M have trace zero, i.e., elements of the Lie algebra $\mathfrak{sl}_n$. As M is skew-symmetric, it is in the Lie algebra $\mathfrak{so}_n$.

For $n = 2$, set $p = p_1 = -p_2$, $q = q_2 = -q_1$ and $Q = e^{-2q}$ such that

$$L = \begin{pmatrix} p & Q \\ Q & -p \end{pmatrix}, \quad M = \begin{pmatrix} 0 & Q \\ -Q & 0 \end{pmatrix}, \quad L(0) = \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix}$$

Consider the solution given by

$$L(t) = \mathrm{Ad}\left[\exp(tL(0))\right]_1^{-1}(L(0))$$

This is motivated by the theory of Lie groups and Lie algebras.

- What is exp?

  It is the exponential of a matrix, i.e.,

$$\exp(A) = e^A = I + A + \frac{A^2}{2!} + \cdots$$

- What is Ad?

  It is the map given by

$$\mathrm{Ad}(A) : M_n(\mathbb{R}) \to M_n(\mathbb{R}), \quad \mathrm{Ad}(A)(V) = AVA^{-1}.$$

  It is an invertible linear map.

- What is the subscript 1?

  Any $A \in M_n(\mathbb{R})$ with $\det A = 1$ can be written uniquely as

$$A = BC, \qquad BB^t = I_n, \qquad \det B = 1$$

  and C is lower triangular with positive entries on the diagonal. We set $A_1 = B$.

In our case, we have the following:

- What is exp?

$$\begin{aligned}\exp(tL(0)) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + t\begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix} + \frac{t^2}{2!}\begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix}^2 + \cdots \\ &= \begin{pmatrix} \cosh(tv) & \sinh(tv) \\ \sinh(tv) & \cosh(tv) \end{pmatrix}\end{aligned}$$

- What is the subscript 1?

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \left[\frac{1}{\sqrt{b^2+d^2}}\begin{pmatrix} d & b \\ -b & d \end{pmatrix}\right]\left[\frac{1}{\sqrt{b^2+d^2}}\begin{pmatrix} 1 & 0 \\ ab+cd & b^2+d^2 \end{pmatrix}\right]$$

$$\exp(tL(0))_1 = \frac{1}{\sqrt{\cosh^2(tv)+\sinh^2(tv)}}\begin{pmatrix} \cosh(tv) & \sinh(tv) \\ -\sinh(tv) & \cosh(tv) \end{pmatrix}$$

- What is $\mathrm{Ad}(A)^{-1}$?

  Note that

  $$\big(\mathrm{Ad}(A^{-1}) \circ \mathrm{Ad}(A)\big)(V) = \mathrm{Ad}(A^{-1})(AVA^{-1}) = V.$$

  Thus, $\mathrm{Ad}(A)^{-1} = \mathrm{Ad}(A^{-1})$.

Putting it all together, we obtain

$$\begin{aligned} L(t) &= \exp(tL(0))_1^{-1} L(0) \exp(tL(0))_1 \\ &= \frac{v}{\cosh(2tv)} \begin{pmatrix} -\sinh(2tv) & 1 \\ 1 & \sinh(2tv) \end{pmatrix} \end{aligned}$$

Therefore, $e^{-2q(t)} = Q(t) = v/\cosh(2tv)$ and

$$q(t) = -\tfrac{1}{2}\ln v + \tfrac{1}{2}\ln(\cosh(2tv))$$

Theorem

There is an explicit solution for the Lax equation for any n given by

$$L(t) = \mathrm{Ad}(\exp(tL(0))_1)^{-1}(L(0)).$$

This involves τ-functions and more Lie theory.

Lax pairs and Lax equation were introduced by Peter Lax (1968) to analyze solitions in continuous media.

Further Remarks

- What about an infinite 1D lattice?
  1974 Flaschka: Solved the infinite 1D lattice (Hilbert spaces, unitary operators)
- What about closed 1D lattices?
  1973 Ford et. al.: 3 particles in a ring with equal masses
- What about integrability?
  1974 Moser: Yes, for the Toda 1D lattice
  1974 Flaschka: Yes, for the infinite 1D lattice
  1974 Hénon: Yes, for the closed 1D lattice
- Do 1D crystals exist?
  2014 Senga, Komsa et. al.: Created a "one dimensional" crystal by packing Cesium Iodide (CsI) inside a carbon nanotube.