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Toda lattice invariants and the Harper's Hamiltonian thermodynamics

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Abstract. A connection between the Toda lattice additive integrals of motion and the Harper's Hamiltonian thermodynamics is established. The Harper's Hamiltonian is shown to be a special case of the Lax operator for the Toda lattice.

1. Introduction

The study of the Harper's Hamiltonian has a rich history, and began with the early work of [1, 2]. In the numerical work by Hofstadter, a fractal nature of the spectrum was discovered [3]. Apart from numerical computations, plenty of different mathematical methods have been applied: quasiclassical WKB [4, 5] and instanton [6] approaches, renormalization group [7] and C^* algebra [8] methods, etc. Recent interest in the model stems from a possible application to a study of superconducting networks [9], wire networks [10], the lattice Ginzburg–Landau theory of superconductivity near the upper critical magnetic field [11], anyon superconductivity [12], organic conductors [13], the quantum Hall effect [14], etc.

Most of the work dedicated to a study of the Harper's model is directed to a calculation of all eigenstates of the operator. But for a physicist this is too detailed for the great majority of cases. More than that, sometimes it is not easy to use effectively such a large amount of information. All physicists need is a calculation of traces, determinants and other invariants which can be used for a computation of observables. The aim of this work is to develop an approach to the Harper's Hamiltonian giving the possibility of a direct calculation of observables without obtaining eigenvalues and eigenvectors.

2. Spectral characteristics of an operator and observables

The Epstein zeta function $\zeta_H(s)$ of an operator H is determined as follows [15]:

$$\zeta_H(s)=\sum_n \lambda_n^{-s} \tag{1}$$

where λ_n are eigenvalues of the operator H,

$$H\phi_n = \lambda_n \phi_n. \tag{2}$$

The one-loop fluctuation correction to a classical free energy functional with the kinetic term $\phi^* H \phi$ [10]

$$\delta F = -(1/2)\ \mathrm{tr}\ \log(H + \tau) \tag{3}$$

can be expressed as [15]

$$\delta F = -\zeta'_H(0). \tag{4}$$

On the other hand, the quantum partition function or the theta function of the operator H is determined as

$$\Theta_H(\beta) = \mathrm{tr}\ \rho = \sum_n \exp(-\beta \lambda_n) \tag{5}$$

where the density matrix ρ satisfies the Bloch equation

$$\partial\rho/\partial\beta = -H\rho. \tag{6}$$

In accordance with Minakshisundaram's theorem [16],

$$\zeta_H(s) = \Gamma^{-1}(s) \int_0^\infty \mathrm{d}\beta\ \beta^{s-1}\ \mathrm{tr}\ \rho(\beta) \tag{7}$$

where $\Gamma(s)$ is the gamma function. Thus we see that the fluctuation correction to the classical free energy (3) and the quantum partition function (5) are linked by the common Epstein zeta function. Comparing (4), (5) and (7) we can write

$$\delta F = -\lim_{s\to 0} \mathrm{d}/\mathrm{d}s\ \Gamma^{-1}(s) \int_0^\infty \mathrm{d}t\ t^{s-1}\ \mathrm{tr}(\rho(x, x, t) - \rho_0(x, x, t)). \tag{8}$$

Here ρ is the density matrix or the thermal kernel of the operator satisfying (6); ρ_0 is a regulator. The theta function of the operator has the asymptotic high-temperature expansion [15]

$$\Theta_H(\beta) = (4\pi\beta)^{-d/2}(a_0 + a_1\beta + \ldots) \tag{9}$$

where a_i are Seeley coefficients [15]; d is the space dimension. In the important and rather generic case we are interested by ultraviolet divergences (small t in (10)); therefore, in this case only a few first Seeley coefficients are necessary. Apart from the thermodynamics written above, formulae can be applied to a calculation of spectral characteristics of the operator. For instance, the density of states

$$g(\lambda) = \sum_n \delta(\lambda - \lambda_n) \tag{10}$$

can be written in the following form:

$$g(\lambda) = (2\pi)^{-1}\ \mathrm{d}/\mathrm{d}\lambda\ \mathrm{tr}\ \log[(H - \lambda + \mathrm{i}O)/(H - \lambda - \mathrm{i}O)]. \tag{11}$$

Our goal now is to express these values in terms of the Toda lattice invariants in the case of the Harper's operator.

3. Connection between the Toda lattice problem and the Harper's Hamiltonian

(i) The equation of motion for the Toda lattice can be written as [16]

$$\mathrm{d}Q_n/\mathrm{d}t=P_n \qquad \mathrm{d}P_n/\mathrm{d}t=\exp[-(Q_n-Q_{n-1})]-\exp[-(Q_{n+1}-Q_n)] \tag{12}$$

or, introducing new variables,

$$a_n=\tfrac{1}{2}\exp[-(Q_{n+1}-Q_n)] \qquad b_n=\tfrac{1}{2}P_n \tag{13}$$

we have

$$\mathrm{d}a_n/\mathrm{d}t=a_n(b_n-b_{n+1}) \qquad \mathrm{d}b_n/\mathrm{d}t=2(a_{n+1}^2-a_n^2). \tag{14}$$

Equations (14) can be written in the matrix form as

$$\mathrm{d}L/\mathrm{d}t=BL-LB \tag{15}$$

or, equivalently, as

$$L(t)=U(t)L(O)U^{-1}(t) \tag{16}$$

where the unitary matrix $U(t)$ evolves according to the equation

$$\mathrm{d}U/\mathrm{d}t=BU(t). \tag{17}$$

Therefore, $L(t)$ is unitary equivalent to $L(O)$ [16]. For a periodic Toda lattice with the boundary conditions

$$a_n=a_{n+N} \qquad b_n=b_{n+N} \tag{18}$$

matrices L and B can be written as

$$L=\begin{vmatrix} b_1 & a_1 & 0 & \dots & 0 & a_N \\ a_1 & b_2 & a_2 & 0 & \dots & 0 \\ 0 & a_2 & b_3 & a_3 & 0 & \dots \\ \vdots & & & \ddots & & 0 \\ 0 & & & & b_{N-1} & a_{N-1} \\ a_N & 0 & \dots & & a_{N-1} & b_N \end{vmatrix}$$

$$B=\begin{vmatrix} 0 & -a_1 & 0 & \dots & & & a_N \\ a_1 & 0 & -a_2 & 0 & \dots & & \\ 0 & a_2 & 0 & -a_3 & & & \\ 0 & & & & & 0 & -a_{N-1} \\ -a_N & & & & & a_{N-1} & 0 \end{vmatrix}. \tag{19}$$

One of the most important properties of the model is that the eigenvalues of the Lax operator are integrals of motion:

$$\mathrm{d}\lambda/\mathrm{d}t=0. \tag{20}$$

This means that the determinant $\det(\lambda I-L)$ is invariant too. It can be expanded as [16]

$$\det(L-\lambda I)=\lambda^N+\lambda^{N-1}I_1+\ldots+\lambda I_{N-1}+I_N \tag{21}$$

where the coefficients I_l are polynomials in a_n and b_n or of the dynamical variables P_n and Q_n. The roots of the equation

$$\det(L-\lambda I)=0 \tag{22}$$

are eigenvalues of the Lax operator L. One can see from (21) that all I_l are constants:

$$\mathrm{d}I_l/\mathrm{d}t=0. \tag{23}$$

They are simply the integrals of motion first found by Hénon [17]. Now we have the necessary minimum of information concerning the Toda lattice to consider our problem.

(ii) The Harper's Hamiltonian appeared for the first time in the study of Landau level splitting and widening due to the lattice symmetry of a crystal potential [1, 2]. It can be written in the form

$$\begin{aligned} H\psi=&\exp(\mathrm{i}\gamma_1(m,n))\psi(m+1,n)+\exp(-\mathrm{i}\gamma_1(m-1,n))\psi(m-1,n)\\ &+\exp(\mathrm{i}\gamma_2(m,n))\psi(m,n+1)+\exp(-\mathrm{i}\gamma_2(m,n-1))\psi(m,n-1) \end{aligned} \tag{24}$$

where

$$\gamma_1(m,n)=(e/bc)\int_{m,n}^{m+1,n} A_i\,\mathrm{d}x_i \qquad \gamma_2(m,n)=(e/bc)\int_{m,n}^{n,n=1} A_i\,\mathrm{d}x_i. \tag{25}$$

Uniformity of the magnetic field transforms the gauge invariance into the following simple constraint [18]:

$$\gamma_1(m,n)+\gamma_2(m+1,n)-\gamma_1(m,n+1)-\gamma_2(m,n)=2\pi(\phi/\phi_0)=\alpha \tag{26}$$

where $\phi_0=(hc)/e$ is the quantum of flux and ϕ is a flux through a plaquette. In the Landau gauge $\gamma(m,n)=0$, $\gamma(m,n)=\alpha m$. Then the lattice translation operator T_n corresponding to the non-magnetic translation in the y-direction on the one plaquette commutes with the Hamiltonian. Thus the solution of the Schrödinger equation factorizes:

$$\psi(m,n)=\exp(\mathrm{i}km)\phi(n) \tag{27}$$

where $k=pa$ with p being a quasi-wave vector component and a being the lattice spacing. The function $\phi(n)$ satisfies the well known Harper's ('almost Mathieu') equation

$$\phi(n+1)+\phi(n-1)+2\cos(\alpha n+k)\phi(n)=E\phi(n). \tag{28}$$

(iii) The central idea of this work is the following observation: the Harper's Hamiltonian written in the matrix form is a special case of the Lax operator L for the Toda lattice with

$$a_n=1 \qquad b_n=2\cos(\alpha n+k). \tag{29}$$

If $\phi/\phi_0=p/q$ with p and q being whole numbers, L is a $q\times q$ matrix.

4. Expression of the Harper's Hamiltonian determinant in terms of Hénon's invariants

The matrix elements of the Harper Hamiltonian determined by (29) have to be considered as the initial conditions for the Toda evolution equations.

Notice that the 'time' parameter t is connected with the evolution equations (14) and (15) and has nothing to do with the non-stationary Schrödinger equation $H\psi = i\,\partial\psi/\partial t$, where $H = L$. The determinant of the matrix $(2L - 2\lambda I)$ can be written as [16]

$$J = \det(2L - 2\lambda I) = \exp\left(-\sum_{k=1}^{N-1} A_k\,\partial^2 \Big/ (\partial B_k\,\partial B_{k+1})\right)\prod_{l=1}^{N}(B_l - 2\lambda) \tag{30}$$

where I is the identity matrix, $N = q$,

$$B_j = 2b_j \qquad A_j = (2a_j)^2. \tag{31}$$

Isospectral deformations due to the evolution equation do not change the spectral invariants and, therefore, we may calculate the determinant (30) with initial values of B_k, A_k.

The wanted $\log\det(L - \lambda I)$ differs from the value $\log J$ by an unimportant additive constant. On the other hand, J can be expanded into a series which stops at the Nth step if p and q are whole numbers:

$$J = (2\lambda)^N + I_1(2\lambda)^{N-1} + \ldots + I_N \tag{32}$$

where I_n is the nth Hénon's integral of motion,

$$I_n = \left(\sum_{j=1}^{N} \partial \Big/ \partial B_j\right)^{N-n} \exp\left(-\sum_{k=1}^{N-1} A_k\,\partial^2 \Big/ (\partial B_k\,\partial B_{k+1})_{l=1}\right)^{N} \prod B_l. \tag{33}$$

Substituting into (32) and (33) the formulae for A_n and B_n (see (31)) and taking into account (29), we have our problem formally solved. Connections between J and other values of interest are given in section 2.

We conclude that the established connection between the Harper's Hamiltonian and the Toda lattice can be used for calculation of spectral and thermodynamic values relevant to this operator. As an example of a physical problem which can be effectively solved with the method suggested here, we can mention the problem of the fluctuation corrections to the free energy of the lattice Landau–Ginzburg model with a background magnetic field, considered using rather rough approximations in [11].

An investigation of the case of irrational α seems to be of particular interest. This study is now in progress.

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