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J. Phys. A: Math. Gen. 28 (1995) 7089–7096. Printed in the UK

On a class of inhomogeneous Ising quantum chains

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Received 24 July 1995

Abstract. The Hamiltonian of an Ising quantum chain with a square-root-increasing transverse magnetic field is exactly diagonalized and its spectrum determined by the zeros of Charlier polynomials. We compute also the magnetization at zero temperature as a function of the position in closed form.

Introduction

Inhomogeneous bidimensional systems have attracted renewed interest in recent years as they have been shown to have unusual critical behaviour [1]. A standard microscopic modelling of such systems is provided by Ising models with non-homogeneous couplings which simulate the presence of defects in the bulk; the parameters of the defect become parameters in critical exponents [2].

Inhomogeneous Ising models are frequently studied in the so-called 'strong anisotropic' limit, in which a Hamiltonian operator for an inhomogeneous quantum spin chain emerges in the form

$$H_N = -\left\{\sum_{n=1}^{N-1} \mu_n \sigma_n^z + \sum_{n=0}^{N-1} \lambda_n \sigma_n^x \sigma_{n+1}^x\right\} \tag{1}$$

where $N+1$ is the number of sites of the chain, σ_n^z, σ_n^x are Pauli matrices at site n, and μ_n is the variable magnetic field and λ_n the inhomogeneous coupling constant.

The homogeneous version of (1) was studied long ago [3], and inhomogeneous chains are of recent concern [1].

There is an interesting context in which H_N of (1) occurs as a geometrical effect on homogeneous Ising models bounded by a contour when one takes the 'strong anisotropic' limit of the lattice.

This is the case of a corner of an Ising model limited by two straight lines meeting at the origin of a coordinate system. Then one obtains an H_N with [4]

$$\mu_n = 2n \qquad \text{and} \qquad \lambda_n = \lambda(2n+1). \tag{2}$$

If one takes the boundary as a parabola of equation $y^2 = Cx$, the resulting H_N is [1]

$$\mu_n = \sqrt{2n} \qquad \text{and} \qquad \lambda_n = \lambda\sqrt{n+1}. \tag{3}$$

More generally for a boundary of equation $y = Cx^\alpha$, one expects the following coefficients [5]:

$$\mu_n = (2n+\mu)^\alpha \qquad \text{and} \qquad \lambda_n = \lambda(2n+1+\mu)^\alpha \tag{4}$$

where μ is a constant.

An alternative way of obtaining H_N would be via the combining of geometrical and physical effects by taking a corner Ising model in the presence of an extended defect [6] of a precise type. This yields

$$\mu_n = 2n \qquad \text{and} \qquad \lambda_n = \lambda(2n+1+\gamma) \tag{5}$$

where γ describes the 'strength' of the defect.

Thus the H_N of interest here exhibits smooth and parallel growth behaviour for both μ_n and λ_n.

In this paper, we follow an idea of Smith [7] who considers only a growing magnetic field for an XY quantum chain with the Hamiltonian

$$H_N^{XY} = -\left\{\sum_{n=0}^{N-1} \lambda(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y) + \sum_{n=1}^{N-1} \mu_n\sigma_n^z\right\} \tag{6}$$

with $\mu_n = Rn + H$, where R and H are constant, and proposed studying an Ising quantum chain with a square-root-growing magnetic field, i.e.

$$H_N = -\left\{\sum_{n=1}^{N-1} \sqrt{n}\sigma_n^z + \lambda \sum_{n=0}^{N-1} \sigma_n^x\sigma_{n+1}^x\right\}. \tag{7}$$

Physically this Hamiltonian may be obtained from the 'strong anisotropic' limit of an Ising model bounded by a parabola as in [1], but containing a Hilhorst–Van Leuween horizontal inhomogeneous coupling of the form $\lambda(n+1)^{-1/2}$ [8]. Thus this is another instance of combined geometrical and physical effects in the bulk. This increasing magnetic field tends to line up the spins of the bulk as one goes away from the origin; one expects that the magnetization grows as function of the distance. Such behaviour has been already found in the work of Smith [7].

1. The method of Lieb, Schultz and Mattis

A general feature of the Hamiltonians H_N is that they may be diagonalized by the method of Lieb, Schultz and Mattis [9]. In their seminal work, they showed that the H_N may be expressed as a bilinear form in fermion variables c_n^+, c_n through the Jordan–Wigner transformation. The fermionic form is in turn diagonalized by a Bogoliubov–Valatin transformation, which gives the normal-mode fermions η_k^+, η_k and their single-mode eigenenergy ε_k.

Following this standard procedure, H_N appears now as

$$H_N = -\sum_{n=1}^{N-1} \sqrt{n}(2c_n^+c_n - 1) - \lambda\sum_{n=0}^{N-1}(c_n^+ - c_n)(c_{n+1}^+ + c_{n+1}). \tag{8}$$

This is a bilinear fermionic form of the type

$$H_N = \sum_{m,n}\{c_m^+A_{mn}c_n + \tfrac{1}{2}(c_m^+B_{mn}c_n^+ + \text{HC})\} + \text{constant} \tag{9}$$

in which A (B) is a real symmetric (antisymmetric) tridiagonal $(N+1)\times(N+1)$ matrix.

To diagonalize H_N, one introduces the normal-mode fermion operators η_k^+, η_k through the relations

$$\eta_k^+ + \eta_k = \sum_{m=0}^{N} \phi_m(k)(c_m^+ + c_m) \qquad \eta_k^+ - \eta_k = \sum_{m=0}^{N} \psi_m(k)(c_m^+ - c_m) \tag{10}$$

and requires that the conditions

$$\sum_{m=0}^{N}(A_{nm}-B_{nm})\psi_m(k)=\varepsilon_k\phi_n(k) \qquad \sum_{m=0}^{N}(A_{nm}+B_{nm})\phi_m(k)=\varepsilon_k\psi_n(k) \tag{11}$$

be obeyed by the coefficients $\phi_m(k)$ and $\psi_m(k)$ so that H_N takes the diagonal form

$$H_N=\sum_{k=0}^{N}\varepsilon_k\eta_k^+\eta_k+\text{constant}. \tag{12}$$

The conditions (11) state merely that $\phi(k)$ and $\psi(k)$ are eigenvectors of a coupled matrix eigenvalue of the problem, which, for practical purposes may be reformulated as

$$(A-B)(A+B)\phi(k)=\varepsilon_k^2\phi(k) \qquad (A+B)(A-B)\psi(k)=\varepsilon_k^2\psi(k) \tag{13}$$

together with the normalization conditions

$$\sum_{n=0}^{N}\phi_n^2(k)=\sum_{n=0}^{N}\psi_n^2(k)=1. \tag{14}$$

2. Diagonalization with Charlier polynomials

The structure of the Hamiltonian (7) is such that the matrices $(A\mp B)(A\pm B)$ are real symmetric tridiagonal $(N+1)\times(N+1)$ matrices. The first equation of (13) may be in fact rewritten as a three-way recursion relation for the $\phi_n(k)$:

$$\lambda\sqrt{n-1}\phi_{n-1}(k)+(n+\lambda^2)\phi_n(k)+\lambda\sqrt{n}\phi_{n+1}(k)=\omega_k^2\phi_n(k) \tag{15}$$

with $\varepsilon_k^2=(2\omega_k)^2$ and $n=2,3,\ldots,N-1$. For $n=0$, 1 and N we have the boundary conditions

$$0\times\phi_0(k)=\omega_k^2\phi_0(k) \tag{16}$$

$$(1+\lambda^2)\phi_1(k)+\lambda\phi_2(k)=\omega_k^2\phi_1(k) \tag{17}$$

$$\lambda\sqrt{N-1}\phi_{N-1}(k)+\lambda^2\phi_N(k)=\omega_k^2\phi_N(k). \tag{18}$$

Similarly the second equation of (13) is a three-way recursion for the $\psi_n(k)$ with three additional boundary conditions:

$$\lambda\sqrt{n}\psi_{n-1}(k)+(n+\lambda^2)\psi_n(k)+\lambda\sqrt{n+1}\psi_{n+1}(k)=\omega_k^2\psi_n(k) \tag{19}$$

$$\lambda^2\psi_0(k)+\sqrt{1}\lambda\psi_1(k)=\omega_k^2\psi_0(k) \tag{20}$$

$$\sqrt{N-1}\lambda\psi_{N-2}(k)+(N-1+\lambda^2)\psi_{N-1}(k)=\omega_k^2\psi_{N-1}(k) \tag{21}$$

$$0\times\psi_N(k)=\omega_k^2\psi_N(k). \tag{22}$$

Relations (15) and (19) may be transformed using the substitutions

$$\phi_n(k)=Q(k)\frac{\lambda^n}{\sqrt{(n-1)!}}q_n(k) \qquad \psi_n(k)=P(k)\frac{\lambda^n}{\sqrt{n!}}p_n(k) \tag{23}$$

($Q(k)$ and $P(k)$ are normalization constants to be determined later) into the following relations:

$$\begin{aligned} q_{n+1}(k)&=\left(\frac{\omega_k^2-1}{\lambda^2}-\frac{n-1}{\lambda^2}-1\right)q_n(k)-\frac{n-1}{\lambda^2}q_{n-1}(k)\\ p_{n+1}(k)&=\left(\frac{\omega_k^2}{\lambda^2}-\frac{n}{\lambda^2}-1\right)p_n(k)-\frac{n}{\lambda^2}p_n(k)\end{aligned} \tag{24}$$

which are typical recursion relations for Charlier polynomials [10]: $C_n(x, \lambda^2)$. Hence we have

$$q_n(k) = C_{n-1}(\omega_k^2 - 1, \lambda^2) \qquad p_n(k) = C_n(\omega_k^2, \lambda^2). \tag{25}$$

The Charlier polynomials $C_n(x, \lambda^2)$ have the explicit expression

$$C_n(x, \lambda^2) = \sum_{\nu=0}^{n} (-1)^{n-\nu} \binom{n}{\nu} \binom{x}{\nu} \nu! \frac{1}{\lambda^{2\nu}}. \tag{26}$$

They enjoy a 'duality' symmetry for $x = k$, an integer:

$$(-1)^k C_n(k, \lambda^2) = (-1)^n C_k(n, \lambda^2) \tag{27}$$

and are orthogonal with respect to the Poisson measure:

$$\sum_{k=0}^{\infty} \mathrm{e}^{-\lambda^2} \frac{\lambda^{2k}}{k!} C_n(k, \lambda^2) C_m(k, \lambda^2) = \frac{n!}{\lambda^{2n}} \delta_{mn} \tag{28}$$

for $m, n = 0, 1, 2, \ldots, \infty$. Combining (27) and (28), one obtains the so-called dual orthogonality relation of Eagleson [11], which holds also for Gottlieb and Hahn polynomials:

$$\sum_{k=0}^{\infty} \mathrm{e}^{-\lambda^2} \frac{\lambda^{2k}}{k!} C_k(n, \lambda^2) C_k(m, \lambda^2) = \frac{n!}{\lambda^{2n}} \delta_{mn}. \tag{29}$$

3. Determination of the spectrum in the limit $N \longrightarrow \infty$

First of all, there exists a zero mode with $\omega_0 = 0$. Equations (14)–(22) yield readily the solutions

$$\phi_n(0) \approx \delta_{n,0} \qquad \text{and} \qquad \psi_n(0) \approx \delta_{N,n}. \tag{30}$$

The rest of the spectrum may be determined by the end of the chain boundary condition (see equation (18)) or its equivalent:

$$N C_{N-1}(\omega_k^2 - 1, \lambda^2) + \lambda^2 C_N(\omega_k^2 - 1, \lambda^2) = 0. \tag{31}$$

Using the asymptotic form of $C_n(x, \lambda^2)$ given by Gottlieb [12] for $n \longrightarrow \infty$:

$$C_n(x, \lambda^2) \approx \frac{\mathrm{e}^{\lambda^2}}{\lambda^{2n}} \frac{\Gamma(1+x)}{\Gamma(1+x-n)} \tag{32}$$

in (31) we obtain

$$\frac{1}{\Gamma(\omega_k^2 - N)} \frac{\omega_k^2}{\omega_k^2 - N} = 0 \tag{33}$$

which, in view of the poles of the Γ function, yields the spectrum in the limit $N \longrightarrow \infty$:

$$\varepsilon_k = -2\sqrt{k} \qquad k = 1, 2, \ldots, \infty. \tag{34}$$

The negative sign is chosen in order to agree with the difference equation satisfied by the Charlier polynomials (see equation (40)).

The boundary condition for $\psi_n(k)$ given in equation (21) may be replaced, using equation (19), by the simpler one for $k \neq 0$:

$$\sqrt{N} \lambda \psi_N(k) = 0 \tag{35}$$

or equivalently, in the $N \longrightarrow \infty$ limit:

$$P(k) \frac{\mathrm{e}^{\lambda^2}}{\lambda^{2N}} \frac{\Gamma(1+\omega_k^2)}{\Gamma(1+\omega_k^2 - N)} = 0. \tag{36}$$

Thus the spectrum found in equation (34) is perfectly consistent with equation (36) in the thermodynamic limit of the chain.

Lastly we may use the Charlier polynomial orthogonality to compute the constants $Q(k)$ and $P(k)$ of the normalized wavefunctions $\phi_n(k)$ and $\psi_n(k)$:

$$\begin{aligned}\psi_n(k) &= e^{-\lambda^2/2}\frac{\lambda^k}{\sqrt{k!}}\frac{\lambda^n}{\sqrt{n!}}C_n(k,\lambda^2)\\ \phi_n(k) &= e^{-\lambda^2/2}\frac{\lambda^{k-1}}{\sqrt{(k-1)!}}\frac{\lambda^{n-1}}{\sqrt{(n-1)!}}C_{n-1}(k-1,\lambda^2).\end{aligned} \tag{37}$$

A completeness relation for $\phi_n(k)$, which is defined for sites $n \gg 1$, is derived in the form

$$\sum_{k=1}^{\infty}\phi_{n+1}(k)\phi_{m+1}(k) = \delta_{mn} \tag{38}$$

with $n, m = 0, 1, 2, \ldots, \infty$. Since $\psi_n(k) = \phi_{n+1}(k+1)$, we also have

$$\sum_{k=1}^{\infty}\psi_n(k)\psi_m(k) = \delta_{mn} \tag{39}$$

for $n, m = 0, 1, 2, \ldots, \infty$. Recall that $\psi_n(0) = \delta_{0\infty}$.

Equations (13) combined with the dual symmetry relation (27) reduce to the difference equation for Charlier polynomials [13]:

$$C_n(k+1,\lambda^2) - C_n(k,\lambda^2) = \frac{n}{\lambda^2}C_{n-1}(k,\lambda^2). \tag{40}$$

As in the past, many of the inhomogeneous one-dimensional Hamiltonians of the free-fermion class (Ising or XY types) [14] are diagonalized with the use of special orthogonal polynomials. But only in this case and in the case of an XX-chain with linearly increasing coupling constant and magnetic field does one get the two classes of dual symmetric polynomials: the Charlier and Gottlieb polynomials. In both cases the spectrum is determined by the zeros of these polynomials.

4. Magnetization profile at $T = 0$ K

Following Smith [7], we compute the magnetization profile at temperature T (or $\beta = 1/kT$):

$$M_m(\beta) = \langle c_m^+ c_m - 1/2\rangle. \tag{41}$$

Inverting (10) by using the orthogonality relations for $\phi_m(k)$ and $\psi_k(k)$, we express the c_m^+ (c_m) in terms of the normal-mode fermions η_k^+ (η_k) (for $m \neq 0$):

$$\begin{aligned}c_m^+ &= \sum_{k=1}^{\infty}\tfrac{1}{2}\{(\phi_m(k)+\psi_m(k))\eta_k^+ + (\phi_m(k)-\psi_m(k))\eta_k\}\\ c_m &= \sum_{k=1}^{\infty}\tfrac{1}{2}\{(\phi_m(k)-\psi_m(k))\eta_k^+ + (\phi_m(k)+\psi_m(k))\eta_k\}.\end{aligned} \tag{42}$$

Then performing the thermal averaging over the η_k^+, η_k:

$$\langle c_m^+ c_m\rangle = \tfrac{1}{4}\sum_{k=1}^{\infty}\frac{1}{(1+e^{\beta\varepsilon_k})}\{(\phi_m(k)+\psi_m(k))^2 + e^{\beta\varepsilon_k}(\phi_m(k)-\psi_m(k))^2\}. \tag{43}$$

Here in the limit of an infinitely long chain the $\varepsilon_k = 2\omega_k$, whereby $\omega_k = -\sqrt{k}$ with $k = 1, 2, \ldots, \infty$. In general because of the Fermi distribution it is difficult to evaluate

$\langle c_m^+ c_m \rangle$ exactly. However, for the given choice of energy sign when $\beta \longrightarrow \infty$ ($T \longrightarrow 0$), we have a simpler expression:

$$M_m(\beta \longrightarrow \infty) = \sum_{k=1}^{\infty} \phi_m(k)\psi_m(k). \tag{44}$$

Using the recursion relation (13) or alternatively (40):

$$\lambda\psi_{m-1}(k) + \sqrt{m}\psi_m(k) = \sqrt{k}\phi_m(k) \tag{45}$$

we obtain

$$M_m(\beta = \infty) = \sum_{k=1}^{\infty} \left\{ \frac{\lambda}{\sqrt{k}}\psi_{m-1}(k)\psi_m(k) + \frac{\sqrt{m}}{\sqrt{k}}\psi_m^2(k) \right\}. \tag{46}$$

Using a bilinear generating function given by Meixner [13], we may write

$$\sum_{k=0}^{\infty} s^k \psi_n(k)\psi_m(k) = (-1)^{n+m}(\sqrt{s})^{n+m} \exp\left(-\frac{\lambda^2}{2}\left(s - \frac{1}{s}\right)\right)(-1)^{(n-m)/2}\psi_m\left(n, -\frac{(1-s)^2\lambda^2}{s}\right) \tag{47}$$

which, despite appearances, is symmetric with respect to the exchange of n and m.

Thus by contour integration around the origin we may extract an identity of the type

$$\begin{aligned}\psi_n(k, \lambda^2)\psi_m(k, \lambda^2) &= \frac{1}{2\mathrm{i}\pi} \oint \frac{\mathrm{d}s}{s^{k+1}} \exp\left(-\frac{\lambda^2}{2}\left(s - \frac{1}{s}\right)\right) \\ &\quad \times (-\sqrt{s})^{n+m}(-1)^{(n-m)/2}\psi_m\left(n, -\frac{(1-s)^2\lambda^2}{s}\right).\end{aligned} \tag{48}$$

We now introduce Jonquière's function:

$$F(z, s) = \sum_{p=1}^{\infty} \frac{z^p}{p^s} \tag{49}$$

and deduce the representation of a kernel in n and m:

$$\begin{aligned}\sum_{k=0}^{\infty} \frac{\psi_n(k, \lambda^2)\psi_m(k, \lambda^2)}{k^\alpha} &= \frac{1}{2\mathrm{i}\pi} \oint \frac{\mathrm{d}s}{s} F\left(\frac{1}{s}, \alpha\right) \exp\left(-\frac{\lambda^2}{2}\left(s - \frac{1}{s}\right)\right) \\ &\quad \times (-\sqrt{s})^{n+m}(-1)^{(n-m)/2}\psi_m\left(n, -\frac{(1-s)^2\lambda^2}{s}\right)\end{aligned} \tag{50}$$

which will be used in computing the magnetization $M_n(\infty)$ at zero temperature, i.e.

$$\begin{aligned}M_m(\beta = \infty) &= \frac{1}{2\mathrm{i}\pi} \oint \frac{\mathrm{d}s}{s} s^m F\left(\frac{1}{s}, \frac{1}{2}\right) \exp\left(-\frac{\lambda^2}{2}\left(s - \frac{1}{s}\right)\right) \\ &\quad \times \left\{ \frac{\mathrm{i}\lambda}{\sqrt{s}}\psi_m(m-1, l) + \sqrt{m}\psi_m(m, l) \right\}\end{aligned} \tag{51}$$

with the parameter

$$l = -\frac{(1-s)^2}{s}\lambda^2. \tag{52}$$

In particular, for $m = 1$, the first site $M_1(\beta = \infty)$ can be evaluated as

$$M_1(\infty) = \mathrm{e}^{-\lambda^2} \sum_{k=0}^{\infty} \frac{\lambda^{2k}}{k!} (\sqrt{k+1} - \sqrt{k}) < 1 \tag{53}$$

because the first two polynomials are simple:

$$C_0(k, \lambda^2) = 1 \qquad \text{and} \qquad C_1(k) = -1 + \frac{k}{\lambda^2}. \tag{54}$$

At the origin the equations determining c_0^+ and c_0 are

$$c_0^+ + c_0 = \eta_0^+ + \eta_0 \qquad c_0^+ - c_0 = \sum_{k=1}^{\infty} \psi_0(k)(\eta_k^+ - \eta_k) \tag{55}$$

since $\phi_n(0) = \delta_{n0}$ and since the completeness relation for the $\psi_n(k)$ is valid down to site $n = 0$. Using

$$\psi_0(k) = \exp\left(\frac{-\lambda^2}{2}\right) \frac{\lambda^k}{\sqrt{k!}} \tag{56}$$

we may compute $\langle c_0^+ c_0 \rangle$ at $T = 0$ and find the magnetization at the origin:

$$M_0 = \left(\langle c_0^+ c_0 \rangle - \frac{1}{2}\right) = -\frac{1}{4}\mathrm{e}^{-\lambda^2}. \tag{57}$$

As the magnetic field is zero at the origin and as $\lambda\sigma_0^x\sigma_1^x$ acts as a spin-flip disordering operator, the first spin tends to be flipped more strongly than the second one which is already under the influence of the magnetic field. As a result the magnetization is negative at the origin but becomes positive at the next site.

Along the chain, the magnetic field will become stronger and stronger whereas the disordering retains a constant strength λ; thus it is expected that M_n will increase steadily and for $n \longrightarrow \infty$ will behave as the magnetization of independent spins in the z-direction.

5. Concluding remarks

The solvability of this Ising Hamiltonian reveals the versatility of free-fermion systems which are somehow related to a very large class of orthogonal polynomials hitherto unrelated to physical problems (e.g. Meixner, Meixner–Pollaczek, and Carlitz polynomials).

Performing a high–low-temperature duality transformation, one may end up considering the dual H_N^* of H_N:

$$H_N^* = -\left\{\sum_{n=1}^{N-1} \lambda\sigma_n^z + \sum_{n=0}^{N-1} \sqrt{n}\sigma_n^x\sigma_{n+1}^x\right\} \tag{58}$$

with constant magnetic field and square-root-increasing coupling constant. The same analysis shows that the three-way recursions for $\phi_n^*(k)$ and $\psi_n^*(k)$ are

$$\begin{aligned} \lambda\sqrt{n-1}\phi_{n-1}^*(k) + (\lambda^2 + n - 1)\phi_n^*(k) + \lambda\sqrt{n}\phi_{n+1}^*(k) &= \omega_k^2\phi_n(k) \\ \lambda\sqrt{n-1}\psi_{n-1}^*(k) + (\lambda^2 + n)\psi_n^*(k) + \lambda\sqrt{n}\psi_{n+1}^*(k) &= \omega_k^2\psi_n(k). \end{aligned} \tag{59}$$

By identification with equations (15) and (19) we get

$$\psi_n^*(k) = \phi_n(k) \qquad \phi_n^*(k) = \psi_{n-1}(k). \tag{60}$$

Hence the dual chain is also solvable with Charlier polynomials.

This study suggests therefore that one should investigate to what extent other orthogonal polynomials may be related to other free-fermion systems.

Acknowledgment

The author thanks L Turban for helpful discussions and comments on the subject.

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