THE INVERSE OF A SEMI-INFINITE SYMMETRIC BANDED MATRIX

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Abstract

We describe a method for obtaining an analytic form for a class of symmetric semi-infinite banded matrices, which are, apart from a finite number of terms, of the Toeplitz type. The results are applied to the determination of the spectrum of two-magnon excitations in Heisenberg spin chains with next-nearest-neighbour interactions.

1 Introduction

A Toeplitz matrix A has elements $A_{\ell,j}$ with the property $A_{\ell,j} = a(\ell - j)$. In the case of semi-infinite matrices ($\ell, j = 0, 1, \ldots$) necessary and sufficient conditions have long been known [1, 2] for the existence of an inverse and for finite matrices the inverse can be computed numerically using the Trench algorithm [3]. The eigen-values and eigen-vectors for the finite symmetric tridiagonal case were obtained by Streater [4]. These results provide an expression for the inverse matrix, which has also been obtained more recently by Hu and O'Connell [5] from a calculation of the determinant and cofactors of the matrix. The method of Hu and O'Connell has been generalised to matrices of bandwidth greater than three by Simons [6]. Similar results have been obtained by Lavis and Southern [7] using a transfer matrix rescaling method which has been utilized for excitations in tight-binding systems [8, 9] and quantum spin chains [10, 11, 12]. In this paper we apply the approach of Lavis and Southern to the problem of inverting a semi-infinite symmetric banded matrix which is, apart from a finite number of terms, of Toeplitz form.

We consider the semi-infinite symmetric banded matrices A of the form[1]

$$\langle \ell|\mathsf{A}|j\rangle = \begin{cases} a(\ell,j) & \text{if } |j-\ell| \le n, \\ 0 & \text{if } |j-\ell| > n, \end{cases} \qquad \ell, j = 0, 1, \ldots, \tag{1}$$

where

$$a(\ell,j) = \mathfrak{a}(|\ell - j|), \qquad \text{when } \ell > \tau \text{ or } j > \tau \text{ (or both).} \tag{2}$$

Without loss of generality let $\mathfrak{a}(n) = 1$.

[1]For any matrix $\boldsymbol{X}$ we denote the row and column vectors formed by its ℓ-th row and j-th column by $\langle \ell|\boldsymbol{X}$ and $\boldsymbol{X}|j\rangle$ respectively and the ℓ, j-th element by $\langle \ell|\boldsymbol{X}|j\rangle$

In section 2 we derive the general form for the inverse of A. In section 3 explicit results are given for bandwidths three and five. The bandwidth five ($n = 2$) results are used in section 4 to obtain the two-magnon spectrum of a generalised spin-S Heisenberg chain and our conclusions are presented in section 5.

2 Method

Given that B is the inverse of A

$$\sum_{m=-n}^{n} a(\ell, \ell+m) b(\ell+m, j) = \delta_{\ell,j}, \tag{3}$$

where $b(\ell, j) = \langle \ell | \mathsf{B} | j \rangle$ if $\ell, j \geq 0$ and zero otherwise, and we have similarly extended the definition (1) so that $a(\ell, j) = 0$ if ℓ or j is negative. We define the $2n$-dimensional vectors

$$\mathbf{b}_\ell(j) = \begin{pmatrix} b(\ell-n+1, j) \\ b(\ell-n+2, j) \\ \vdots \\ b(\ell+n, j) \end{pmatrix}, \tag{4}$$

and the $2n \times 2n$ matrices

$$\mathsf{T}_\ell \quad = \quad \begin{pmatrix} -\dfrac{a(\ell,\ell-n+1)}{a(\ell,\ell+n)} & -\dfrac{a(\ell,\ell-n+2)}{a(\ell,\ell+n)} & \cdots & -\dfrac{a(\ell,\ell+n-1)}{a(\ell,\ell+n)} & -1 \\ 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix}, \tag{5}$$

$$\mathsf{Q}_\ell \quad = \quad \begin{pmatrix} \dfrac{a(\ell,\ell-n)}{a(\ell,\ell+n)} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & 0 & 1 & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & 1 & 0 \\ 0 & 0 & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix}. \tag{6}$$

Then equation (3) can be expressed in the form

$$\mathsf{T}_\ell \mathbf{b}_\ell(j) = \mathsf{Q}_\ell \mathbf{b}_{\ell-1}(j) - \frac{\delta_{\ell,j} \mathsf{I} |1\rangle}{a(j, j+n)}. \tag{7}$$

Iterating (7) gives

$$\mathbf{b}_\ell(j) = \mathbf{\Phi}(\ell, 0) \mathbf{b}_{-1}(j) - \frac{\mathbf{\Phi}(\ell, j)|1\rangle}{a(j, j+n)}, \tag{8}$$

where

$$\mathbf{\Phi}(\ell, m) = \begin{cases} \mathsf{T}_\ell^{-1} \mathsf{Q}_\ell \cdots \mathsf{T}_{m+1}^{-1} \mathsf{Q}_{m+1} \mathsf{T}_m^{-1}, & \text{if } \ell > m, \\ \mathsf{T}_m^{-1}, & \text{if } \ell = m, \\ \mathbf{0}, & \text{if } \ell < m. \end{cases} \tag{9}$$

From equations (2), (5) and (6) we see that, when $\ell > \tau$, (9) gives

$$\mathbf{\Phi}(\ell, m) = \begin{cases} \mathsf{T}^{\tau-\ell} \mathbf{\Phi}(\tau, m), & \tau \geq m, \\ \mathsf{T}^{m-1-\ell}, & m > \tau, \end{cases} \tag{10}$$

where

$$\mathbf{T} = \begin{pmatrix} -\mathfrak{a}(n-1) & -\mathfrak{a}(n-2) & \cdots & -\mathfrak{a}(n-1) & -1 \\ 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix}. \tag{11}$$

In a previous paper [7] two of the authors have showed that

$$\langle p|\mathbf{T}^m|q\rangle = u_q(m-p+1), \qquad p,q = 1,\ldots,2n, \tag{12}$$

where

$$u_q(\mu) = \sum_{r=0}^{2n-q} \mathfrak{a}(|n-q-r|) \sum_{k=1}^{n} \frac{\sin\{(n+\mu-r-1)\theta_k\}}{F'(\theta_k)} \tag{13}$$

and $\pm\theta_1, \pm\theta_2, \ldots, \pm\theta_n$ are the roots of

$$0 = F(\theta) \equiv \cos(n\theta) + \tfrac{1}{2}\mathfrak{a}(0) + \sum_{r=1}^{n-1} \mathfrak{a}(r)\cos(r\theta), \tag{14}$$

with

$$u_q(\mu) = \begin{cases} -u_1(\mu-1), & \text{for } q = 2n, \\ -\mathfrak{a}(|n-q|)u_1(\mu-1) + u_{q+1}(\mu-1), & \text{for } 1 \le q < 2n, \end{cases} \tag{15}$$

$$u_1(\mu) = -u_{2n}(\mu+1) = -\sum_{k=1}^{n} \frac{\sin\{(n+\mu)\theta_k\}}{F'(\theta_k)}. \tag{16}$$

Then, from (10) and (12),

$$\langle p|\mathbf{\Phi}(\ell,m)|q\rangle = \begin{cases} \displaystyle\sum_{r=1}^{2n} u_r(\tau-p-\ell+1)\langle r|\mathbf{\Phi}(\tau,m)|q\rangle, & \ell > \tau \ge m, \\ u_q(m-p-\ell), & \ell \ge m > \tau. \end{cases} \tag{17}$$

The vector $\mathbf{b}_{-1}(j)$ has n zero entries and, from (8),

$$b(\ell,j) = \sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\ell,0)|n+m\rangle b(m-1,j) - \frac{\langle n|\mathbf{\Phi}(\ell,j)|1\rangle}{a(j,j+n)}. \tag{18}$$

Thus all the elements in the j-th column of $\mathbf{B}$ can be expressed as a linear combination of the elements $\langle 0|\mathbf{B}|j\rangle, \langle 1|\mathbf{B}|j\rangle, \ldots, \langle n-1|\mathbf{B}|j\rangle$. Replacing ℓ in (18) by $\kappa\sigma$ for some positive integer σ and $\kappa = 1,2,\ldots,n$ yields the set of equations.

$$b(\kappa\sigma,j) \;=\; \sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\kappa\sigma,0)|n+m\rangle b(m-1,j) - \frac{\langle n|\mathbf{\Phi}(\kappa\sigma,j)|1\rangle}{a(j,j+n)}, \qquad \kappa = 1,2,\ldots,n. \tag{19}$$

We now define the $n\times n$ matrix

$$\mathbf{U}_\sigma = \begin{pmatrix} \langle n|\mathbf{\Phi}(\sigma,0)|n+1\rangle & \langle n|\mathbf{\Phi}(\sigma,0)|n+2\rangle & \cdots & \langle n|\mathbf{\Phi}(\sigma,0)|2n\rangle \\ \langle n|\mathbf{\Phi}(2\sigma,0)|n+1\rangle & \langle n|\mathbf{\Phi}(2\sigma,0)|n+2\rangle & \cdots & \langle n|\mathbf{\Phi}(2\sigma,0)|2n\rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle n|\mathbf{\Phi}(n\sigma,0)|n+1\rangle & \langle n|\mathbf{\Phi}(n\sigma,0)|n+2\rangle & \cdots & \langle n|\mathbf{\Phi}(n\sigma,0)|2n\rangle \end{pmatrix} \tag{20}$$

and, from (19),

$$b(\ell,j) = \sum_{\kappa=1}^{n}\langle\ell+1|\mathbf{U}_\sigma^{-1}|\kappa\rangle b(\kappa\sigma,j)+\frac{1}{a(j,j+n)}\sum_{\kappa=1}^{n}\langle\ell+1|\mathbf{U}_\sigma^{-1}|\kappa\rangle\langle n|\mathbf{\Phi}(\kappa\sigma,j)|1\rangle, \qquad \ell=0,1,\ldots,n-1. \tag{21}$$

We now consider the limit $\sigma\to\infty$. Since the form for $u_q(\mu)$ given by (13) is invariant under the change of sign of the solutions $\theta_1,\ldots,\theta_n$ of (14), we can, by if necessary taking a small imaginary part in $\mathfrak{a}(0)$, suppose that each θ_k has a positive imaginary part. Then

$$\begin{aligned} u_q(\mu-\kappa\sigma) &\simeq \sum_{r=0}^{2n-q}\mathfrak{a}(|n-q-r|)\sum_{k=1}^{n}\frac{\exp\{(n+\mu-\kappa\sigma-r-1)\mathrm{i}\theta_k\}}{2\mathrm{i}F'(\theta_k)} \\ &\sim \exp\left\{\kappa\sigma\max_k[\Im(\theta_k)]\right\}. \end{aligned} \tag{22}$$

Giving

$$\begin{aligned} \langle\ell+1|\mathbf{U}_\sigma^{-1}|k\rangle &\sim \exp\left\{-\kappa\sigma\max_k[\Im(\theta_k)]\right\}, \\ \langle n|\mathbf{\Phi}(k\sigma,j)|1\rangle &\sim \exp\left\{\kappa\sigma\max_k[\Im(\theta_k)]\right\}. \end{aligned} \tag{23}$$

If the inverse of the matrix $\mathbf{A}$ exists then $b(\kappa\sigma,j)$ is bounded in the limit $\sigma\to\infty$ for all κ and j with

$$b(\ell,j) = \frac{1}{a(j,j+n)}\lim_{\sigma\to\infty}\sum_{\kappa=1}^{n}\langle\ell+1|\mathbf{U}_\sigma^{-1}|\kappa\rangle\langle n|\mathbf{\Phi}(\kappa\sigma,j)|1\rangle, \qquad \ell=0,1,\ldots,n-1. \tag{24}$$

For $\ell\geq n$, $b(\ell,j)$ is given by substituting from (24) into (18).

3 Explicit formulae

3.1 The case $\mathbf{n=1}$

In this case $\mathbf{U}_\sigma$ is a 1×1 matrix and, from (18), (20) and (24),

$$b(0,j) = \frac{1}{a(j,j+1)}\lim_{\sigma\to\infty}\frac{\langle 1|\mathbf{\Phi}(\sigma,j)|1\rangle}{\langle 1|\mathbf{\Phi}(\sigma,0)|2\rangle}, \tag{25}$$

$$b(\ell,j) = \langle 1|\mathbf{\Phi}(\ell,0)|2\rangle b(0,j)-\frac{\langle 1|\mathbf{\Phi}(\ell,j)|1\rangle}{a(j,j+1)}. \tag{26}$$

From (16),

$$u_1(\mu)=-u_2(\mu+1)=\mathsf{U}_\mu(\cos(\theta)), \qquad 2\cos(\theta)=-\mathfrak{a}(0), \tag{27}$$

where

$$\mathsf{U}_\mu(\cos(\theta))=\frac{\sin\{(\mu+1)\theta\}}{\sin(\theta)} \tag{28}$$

is the Chebyshev polynomial of the second kind and, from (17),

$$\langle 1|\boldsymbol{\Phi}(\ell,m)|q\rangle = \begin{cases} \dfrac{\sin\{(\tau-\ell+1)\theta\}\langle 1|\boldsymbol{\Phi}(\tau,m)|q\rangle - \sin\{(\tau-\ell)\theta\}\langle 2|\boldsymbol{\Phi}(\tau,m)|q\rangle}{\sin(\theta)}, & \\ & \ell > \tau \geq m,\ q=1,2, \\ \dfrac{\sin\{(m-\ell)\theta\}}{\sin(\theta)}, & \ell \geq m > \tau,\ q=1, \\ -\dfrac{\sin\{(m-\ell-1)\theta\}}{\sin(\theta)}, & \ell \geq m > \tau,\ q=2. \end{cases} \tag{29}$$

Thus, from (25),

$$b(0,j) = \begin{cases} \dfrac{\exp\{\mathrm{i}\theta\}\langle 1|\boldsymbol{\Phi}(\tau,j)|1\rangle - \langle 2|\boldsymbol{\Phi}(\tau,j)|1\rangle}{a(j,j+1)\{\exp\{\mathrm{i}\theta\}\langle 1|\boldsymbol{\Phi}(\tau,0)|2\rangle - \langle 2|\boldsymbol{\Phi}(\tau,0)|2\rangle\}}, & \tau \geq j, \\ \dfrac{\exp\{\mathrm{i}(j-\tau)\theta\}}{a(j,j+1)\{\exp\{\mathrm{i}\theta\}\langle 1|\boldsymbol{\Phi}(\tau,0)|2\rangle - \langle 2|\boldsymbol{\Phi}(\tau,0)|2\rangle\}}, & j > \tau. \end{cases} \tag{30}$$

With $\tau = 0$, A is a tridiagonal semi-infinite Toeplitz matrix with $a(\ell,\ell\pm 1) = 1$, $a(\ell,\ell) = \mathfrak{a}(0)$, except when $\ell = 0$. In this case equations (30) and (26) give

$$b(\ell,j) = \begin{cases} f(\ell,j), & \ell \leq j \\ f(\ell,j) + \dfrac{\sin\{(\ell-j)\theta\}}{\sin(\theta)}, & \ell > j, \end{cases} \tag{31}$$

where

$$f(\ell,j) = -\frac{\exp(\mathrm{i}j\theta)[\sin\{\ell\theta\}a(0,0) + \sin\{(\ell-1)\theta\}]}{\sin(\theta)\{\exp(\mathrm{i}\theta) + a(0,0)\}}. \tag{32}$$

3.2 The case $\mathbf{n = 2}$

In this case U_σ is a 2×2 matrix and, from (20) and (24),

$$b(0,j) = \frac{1}{a(j,j+2)}\lim_{\sigma\to\infty}\frac{\phi(2,2;2\sigma,\sigma;4,1;j)}{\phi(2,2;2\sigma,\sigma;4,3,0)}, \tag{33}$$

$$b(1,j) = -\frac{1}{a(j,j+2)}\lim_{\sigma\to\infty}\frac{\phi(2,2;2\sigma,\sigma;3,1;j)}{\phi(2,2;2\sigma,\sigma;4,3;0)}, \tag{34}$$

where

$$\phi(\ell,m;x,y;p,q;j) = \langle\ell|\boldsymbol{\Phi}(x,0)|p\rangle\langle m|\boldsymbol{\Phi}(y,j)|q\rangle - \langle m|\boldsymbol{\Phi}(y,0)|p\rangle\langle\ell|\boldsymbol{\Phi}(x,j)|q\rangle. \tag{35}$$

From (18),

$$b(\ell,j) = \langle 2|\boldsymbol{\Phi}(\ell,0)|3\rangle b(0,j) + \langle 2|\boldsymbol{\Phi}(\ell,0)|4\rangle b(1,j) - \frac{\langle 2|\boldsymbol{\Phi}(\ell,j)|1\rangle}{a(j,j+2)}. \tag{36}$$

Equation (14) is now a quadratic in the variable $z = \cos(\theta)$ with roots $\mathrm{z}^{(+)}$ and $\mathrm{z}^{(-)}$ given by

$$\mathrm{z}^{(\pm)} = \mathrm{z}(\pm\mathcal{Z}) = \tfrac{1}{4}\{-\mathfrak{a}(1) \pm \mathcal{Z}\}, \tag{37}$$

where

$$\mathcal{Z} = \sqrt{[\mathfrak{a}(1)]^2 + 8 - 4\mathfrak{a}(0)}. \tag{38}$$

We define

$$\mathsf{V}(\ell) = \frac{\mathsf{U}_\ell(\mathrm{z}^{(+)}) - \mathsf{U}_\ell(\mathrm{z}^{(-)})}{2\{\mathrm{z}^{(+)} - \mathrm{z}^{(-)}\}} \tag{39}$$

where, from (28),

$$\mathsf{V}(-\ell) = -\mathsf{V}(\ell-2) \tag{40}$$

and, from (14)–(16),

$$\left.\begin{aligned} u_1(\ell) &= \mathsf{V}(\ell+1), \\ u_2(\ell) &= -2\{1+2\mathsf{z}^{(+)}\mathsf{z}^{(-)}\}\mathsf{V}(\ell) + 2\{\mathsf{z}^{(+)}+\mathsf{z}^{(-)}\}\mathsf{V}(\ell-1) - \mathsf{V}(\ell-2), \\ u_3(\ell) &= 2\{\mathsf{z}^{(+)}+\mathsf{z}^{(-)}\}\mathsf{V}(\ell) - \mathsf{V}(\ell-1), \\ u_4(\ell) &= -\mathsf{V}(\ell). \end{aligned}\right\} \tag{41}$$

We define

$$\begin{aligned} W_\sigma(x,y) \quad = \quad & \mathsf{V}(x+2\sigma-\tau-2)\mathsf{V}(y+\sigma-\tau-2) \\ & -\mathsf{V}(x+\sigma-\tau-2)\mathsf{V}(y+2\sigma-\tau-2). \end{aligned} \tag{42}$$

Then, from (17) and (35), when $\tau \geq j$,

$$\begin{aligned} \phi(2,2;2\sigma,\sigma;p,q;j) \quad = \quad & \mathfrak{C}_{01}(p,q;j)W_\sigma(0,1) + \mathfrak{C}_{02}(p,q;j)W_\sigma(0,2) \\ & +\mathfrak{C}_{03}(p,q;j)W_\sigma(0,3) + \mathfrak{C}_{12}(p,q;j)W_\sigma(1,2) \\ & +\mathfrak{C}_{13}(p,q;j)W_\sigma(1,3) + \mathfrak{C}_{23}(p,q;j)W_\sigma(2,3), \end{aligned} \tag{43}$$

where

$$\left.\begin{aligned} \mathfrak{C}_{01}(p,q;j) &= -\mathfrak{a}(0)\phi(1,2;\tau,\tau;p,q;j) - \mathfrak{a}(1)\phi(1,3;\tau,\tau;p,q;j) \\ &\qquad -\phi(1,4;\tau,\tau;p,q;j), \\ \mathfrak{C}_{02}(p,q;j) &= -\mathfrak{a}(1)\phi(1,2;\tau,\tau;p,q;j) - \phi(1,3;\tau,\tau;p,q;j), \\ \mathfrak{C}_{03}(p,q;j) &= -\phi(1,2;\tau,\tau;p,q;j), \\ \mathfrak{C}_{12}(p,q;j) &= (\mathfrak{a}(0)-\mathfrak{a}(1)^2)\phi(2,3;\tau,\tau;p,q;j) - \mathfrak{a}(1)\phi(2,4;\tau,\tau;p,q;j) \\ &\qquad -\phi(3,4;\tau,\tau;p,q;j), \\ \mathfrak{C}_{13}(p,q;j) &= -\mathfrak{a}(1)\phi(2,3;\tau,\tau;p,q;j) - \phi(2,4;\tau,\tau;p,q;j), \\ \mathfrak{C}_{23}(p,q;j) &= -\phi(2,3;\tau,\tau;p,q;j). \end{aligned}\right\} \tag{44}$$

When $j > \tau$ the form of $\phi(2,2;2\sigma,\sigma;p,q;j)$ differs according to the value of q. However, from (33) and (34), we need only the cases $q = 1$ and $q = 3$ which are given by

$$\begin{aligned} \phi(2,2;2\sigma,\sigma;p,1;j) \quad = \quad & \mathfrak{A}_{01}(p)W_\sigma(0,1+j-\tau) + \mathfrak{A}_{11}(p)W_\sigma(1,1+j-\tau) \\ & +\mathfrak{A}_{21}(p)W_\sigma(2,1+j-\tau) + \mathfrak{A}_{31}(p)W_\sigma(3,1+j-\tau), \end{aligned} \tag{45}$$

where

$$\left.\begin{aligned} \mathfrak{A}_{01}(p) &= \langle 1|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{A}_{11}(p) &= -\mathfrak{a}(0)\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle - \mathfrak{a}(1)\langle 3|\mathbf{\Phi}(\tau,0)|p\rangle - \langle 4|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{A}_{21}(p) &= -\mathfrak{a}(1)\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle - \langle 3|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{A}_{31}(p) &= \langle 2|\mathbf{\Phi}(\tau,0)|p\rangle \end{aligned}\right\} \tag{46}$$

and

$$\begin{aligned} \phi(2,2;2\sigma,\sigma;p,3;j) \quad = \quad & \mathfrak{B}_{02}(p)W_\sigma(0,2+j-\tau) + \mathfrak{B}_{03}(p)W_\sigma(0,3+j-\tau) \\ & +\mathfrak{B}_{12}(p)W_\sigma(1,2+j-\tau) + \mathfrak{B}_{13}(p)W_\sigma(1,3+j-\tau) \\ & +\mathfrak{B}_{22}(p)W_\sigma(2,2+j-\tau) + \mathfrak{B}_{23}(p)W_\sigma(2,3+j-\tau) \\ & +\mathfrak{B}_{32}(p)W_\sigma(3,2+j-\tau) + \mathfrak{B}_{33}(p)W_\sigma(3,3+j-\tau), \end{aligned} \tag{47}$$

where

$$\left.\begin{aligned} \mathfrak{B}_{02}(p) &= -\mathfrak{a}(1)\langle 1|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{03}(p) &= -\langle 1|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{12}(p) &= \mathfrak{a}(0)\mathfrak{a}(1)\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle + \mathfrak{a}(1)^2\langle 3|\mathbf{\Phi}(\tau,0)|p\rangle + \mathfrak{a}(1)\langle 4|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{13}(p) &= \mathfrak{a}(0)\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle + \mathfrak{a}(1)\langle 3|\mathbf{\Phi}(\tau,0)|p\rangle + \langle 4|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{22}(p) &= \mathfrak{a}(1)^2\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle + \mathfrak{a}(1)\langle 3|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{23}(p) &= \mathfrak{a}(1)\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle + \langle 3|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{32}(p) &= \mathfrak{a}(1)\langle 2|\mathbf{\Phi}(\tau,0)|p\rangle, \\ \mathfrak{B}_{33}(p) &= \langle 2|\mathbf{\Phi}(\tau,0)|p\rangle. \end{aligned}\right\} \tag{48}$$

It is not difficult to show that

$$\lim_{\sigma\to\infty}\frac{W_\sigma(x,y)}{W_\sigma(0,1)}=\frac{[\zeta(\mathcal{Z})]^y[\zeta(-\mathcal{Z})]^x-[\zeta(\mathcal{Z})]^x[\zeta(-\mathcal{Z})]^y}{\zeta(\mathcal{Z})-\zeta(-\mathcal{Z})}, \tag{49}$$

where

$$\zeta(\pm\mathcal{Z})=\mathcal{M}[\mathrm{z}(\pm\mathcal{Z})] \tag{50}$$

and

$$\mathcal{M}[\mathrm{z}]\equiv \text{The root of larger magnitude of}\{q^2+2\mathrm{z}q+1=0\}. \tag{51}$$

The possibility of the roots being degenerate in magnitude is, as indicated above, removed by the introduction of a small imaginary part in $\mathfrak{a}(0)$ and thus in $z(\pm\mathcal{Z})$.

4 Two-magnon excitations

The multi-magnon spectra of generalized spin-S Heisenberg chains with nearest-neighbour interactions have recently been studied using scaling [10] and recursion [11] methods. The approach involves expressing the m-magnon Schrödinger equation in tight-binding form. The two- and three-magnon excitations are then obtained using scaling and recursion procedures respectively. The former method can be seen to be an application of the technique used in this paper to invert a semi-infinite symmetric banded matrix. Cyr *et al.* applied the recursion method to obtain the three-magnon spectrum of the next-nearest-neighbour model with Hamiltonian

$$\hat{\mathcal{H}}=-\sum_{i=1}^{N}\{J_1\tilde{S}_i\cdot\tilde{S}_{i+1}+J_2\tilde{S}_i\cdot\tilde{S}_{i+2}+J_3\tilde{S}_{i-1}\cdot(\tilde{S}_i\times\tilde{S}_{i+1})\}, \tag{52}$$

where $\tilde{S}_i$ is the quantum spin located at site i of a uniform chain with lattice spacing a_0 and periodic boundary conditions. They described briefly the use of the scaling method to obtain the two-magnon spectrum indicating that more detail would be provided in another publication. These details can now be given in terms of the analysis of the $n=2$ case given in the preceding section.

The ferromagnetic state with all N spins parallel is an exact eigenstate of (52) with energy $E_0=-NS^2(J_1+J_2)$. We shall study the excitation spectrum of (52) relative to the ferromagnetic state.

The one magnon excitation energy is given by

$$E_1=2S\{J_1+2SJ_3\sin(ka_0)\}\{1-\cos(ka_0)\}+2SJ_2\{1-\cos(2ka_0)\}, \tag{53}$$

where k is a wave-vector in the range $-\pi/a_0\leq k\leq\pi/a_0$. Assuming that $J_1>0$ the condition that $E_1\geq 0$ is that

$$\begin{array}{ll} 1+2\beta+\mathrm{sign}(\beta)\sqrt{4\beta^2+\gamma^2}\geq 0, & \text{if } \beta\neq 0,\\ \gamma\leq 1, & \text{if } \beta=0, \end{array} \tag{54}$$

where $\beta=J_2/J_1$ and $\gamma=2S|J_3|/J1$.

The two-magnon problem is soluble in any dimension, since it is equivalent to a defect problem on a d-dimensional lattice. In $d=1$ Majumdar [13] considered the Hamiltonian in (52) with $J_3=0$ and $S=\frac{1}{2}$ and Bahurmuz and Loly [14] investigated the same problem with $S=\frac{1}{2}$ and $S=1$. The two-magnon excitations are solutions of the Schrödinger equation which can be written in terms of the the basis of two-spin deviation states

$$|i,j\rangle=S_i^+S_j^+|0\rangle,\qquad i\leq j, \tag{55}$$

where $|0\rangle$ represents the ferromagnetic state with all spins aligned in the negative z-direction. Using the translational invariance of the Hamiltonian, a transformation can be performed to a mixed orthonormal basis $|K;\ell\rangle$, where K represents the total wave-vector of the pair and $\ell = |j-i|$ is the relative separation of the spin deviations. In this mixed basis and in the limit $N \to \infty$ the Hamiltonian has the tight-binding form

$$\hat{\mathcal{H}} = \sum_{\ell=0}^{\infty} \{|K;\ell\rangle\varepsilon_\ell\langle K;\ell| + |K;\ell\rangle V_\ell\langle K;\ell+1| + |K;\ell\rangle V'_\ell\langle K;\ell+2|\}, \tag{56}$$

where

$$\left.\begin{array}{ll}
\varepsilon_0 & = 4S(J_1+J_2), \\
\varepsilon_1 & = (4S-1)J_1 + 2SJ_2\{2-\cos(K)\} + 2S(1-S)J_3\sin(K), \\
\varepsilon_2 & = 4SJ_1 + (4S-1)J_2, \\
\varepsilon_\ell & = \varepsilon = 4SJ_1 + 4SJ_2, \qquad \ell \geq 3, \\
V_0 & = -2\sqrt{S(2S-1)}J_1\cos(K/2) + 4SJ_3\sqrt{S(2S-1)}\sin(K/2), \\
V_1 & = -2SJ_1\cos(K/2) + 2S(2S-1)J_3\sin(K/2), \\
V_\ell & = V = -2SJ_1\cos(K/2) + 4S^2J_3\sin(K/2), \qquad \ell \geq 2, \\
V'_0 & = -2\sqrt{S(2S-1)}J_2\cos(K) - 2SJ_3\sqrt{S(2S-1)}\sin(K), \\
V'_\ell & = V' = -2SJ_2\cos(K) - 2S^2J_3\sin(K), \qquad \ell \geq 1.
\end{array}\right\} \tag{57}$$

The Green's function operator $\hat{\mathcal{G}}(E)$ is defined [15], for energy E, by

$$\hat{\mathcal{G}}(E)\{E\hat{\mathcal{I}} - \hat{\mathcal{H}}\} = \hat{\mathcal{I}}. \tag{58}$$

In terms of the tight-binding picture the local density of states at site ℓ is given by

$$\rho_\ell(E) = -\lim_{\delta\to 0+} \frac{\Im\{G_\ell(E+\mathrm{i}\delta)\}}{\pi}. \tag{59}$$

For the two-magnon picture $\rho_\ell(E)$ is the density of the scattering state continuum for two magnons located at sites with a separation of ℓa. Comparing equations (1) and (2) with (56) and (57) we see that the matrix $\mathbf{A}$ with elements

$$a(\ell,j) = -\langle K;\ell|\frac{\{E\hat{\mathcal{I}} - \hat{\mathcal{H}}\}}{V'}|K;j\rangle \tag{60}$$

is of the banded symmetric form with $n=2$, $\tau=2$ and

$$\left.\begin{array}{rl}
a(\ell,\ell) & = \begin{cases} \quad\;\; \mu_\ell - \mathcal{E}, & \ell \leq 2, \\ \mathfrak{a}(0) = \quad -\mathcal{E}, & \ell > 2, \end{cases} \\[2ex]
a(\ell,\ell+1) = a(\ell+1,\ell) & = \begin{cases} \quad\;\; \nu_\ell, & \ell \leq 1, \\ \mathfrak{a}(1) = \nu, & \ell > 1, \end{cases} \\[2ex]
a(\ell,\ell+2) = a(\ell+2,\ell) & = \begin{cases} \nu'_0, & \ell = 0, \\ 1, & \ell > 0, \end{cases}
\end{array}\right\} \tag{61}$$

where

$$\left.\begin{array}{llll}
\mathcal{E} = \dfrac{E-\varepsilon}{V'}, & \mu_\ell = \dfrac{\varepsilon_\ell - \varepsilon}{V'}, & \ell = 0,1,2, & \\[2ex]
\nu = \dfrac{V}{V'}, & \nu_\ell = \dfrac{V_\ell}{V'}, & \ell = 0,1, & \nu'_0 = \dfrac{V'_0}{V'}
\end{array}\right\} \tag{62}$$

and from (37)

$$\mathrm{z}^{(\pm)} = z(\pm\mathcal{Z}(\mathcal{E})) = \tfrac{1}{4}\{-\nu \pm \mathcal{Z}(\mathcal{E})\}, \tag{63}$$

with

$$\mathcal{Z}(\mathcal{E}) = \sqrt{\nu^2 + 8 + 4\mathcal{E}}. \tag{64}$$

With these definitions for the elements of $\mathbf{A}$ the matrix elements of the Green's function are given in terms of the inverse matrix $\mathbf{B}$ by

$$\langle K;\ell|\hat{\mathcal{G}}(\mathcal{E})|K;j\rangle = -\frac{b(\ell,j)}{V'}. \tag{65}$$

In particular the two leading diagonal Green's functions are

$$G_\ell(E) = \langle K;\ell|\hat{\mathcal{G}}(\mathcal{E})|K;\ell\rangle = \frac{1}{V'}\frac{\mathsf{G}^{(\ell)}(\mathcal{E})}{(\mathcal{E}-\mu_\ell)\mathsf{G}^{(\ell)}(\mathcal{E}) + \mathsf{F}^{(\ell)}(\mathcal{E})}, \quad \ell = 0,1, \tag{66}$$

where

$$\begin{aligned}
\mathsf{F}^{(\ell)}(\mathcal{E}) &= \mathsf{f}_{01}^{(\ell)}(\mathcal{E}) + \mathsf{f}_{02}^{(\ell)}(\mathcal{E})A(\mathcal{E}) + \mathsf{f}_{03}^{(\ell)}(\mathcal{E})\{[A(\mathcal{E})]^2 - B(\mathcal{E})\} + \mathsf{f}_{12}^{(\ell)}(\mathcal{E})B(\mathcal{E}) \\
&\quad + \mathsf{f}_{13}^{(\ell)}(\mathcal{E})A(\mathcal{E})B(\mathcal{E}) + \mathsf{f}_{23}^{(\ell)}(\mathcal{E})[B(\mathcal{E})]^2, \qquad (67) \\
\mathsf{G}^{(\ell)}(\mathcal{E}) &= \mathsf{g}_{01}^{(\ell)}(\mathcal{E}) + \mathsf{g}_{02}^{(\ell)}(\mathcal{E})A(\mathcal{E}) + \mathsf{g}_{03}^{(\ell)}(\mathcal{E})\{[A(\mathcal{E})]^2 - B(\mathcal{E})\} + \mathsf{g}_{12}^{(\ell)}(\mathcal{E})B(\mathcal{E}) \\
&\quad + \mathsf{g}_{13}^{(\ell)}(\mathcal{E})A(\mathcal{E})B(\mathcal{E}) + \mathsf{g}_{23}^{(\ell)}(\mathcal{E})[B(\mathcal{E})]^2, \qquad (68)
\end{aligned}$$

$$\left.\begin{aligned}
A(\mathcal{E}) &= \zeta(\mathcal{Z}(\mathcal{E})) + \zeta(-\mathcal{Z}(\mathcal{E})), \\
B(\mathcal{E}) &= \zeta(\mathcal{Z}(\mathcal{E}))\zeta(-\mathcal{Z}(\mathcal{E})).
\end{aligned}\right\} \tag{69}$$

$$\left.\begin{aligned}
\mathsf{f}_{01}^{(0)}(\mathcal{E}) &= \nu_0'^2, \qquad \mathsf{f}_{02}^{(0)}(\mathcal{E}) = \nu_0'\nu_0, \qquad \mathsf{f}_{03}^{(0)}(\mathcal{E}) = 0, \\
\mathsf{f}_{12}^{(0)}(\mathcal{E}) &= \nu_0'^2(\mathcal{E}-\mu_1) - \nu_0\nu_0'(\nu - 2\nu_1) - \nu_0^2\mu_2, \\
\mathsf{f}_{13}^{(0)}(\mathcal{E}) &= -\nu_0\nu_0', \qquad \mathsf{f}_{23}^{(0)}(\mathcal{E}) = -\nu_0^2,
\end{aligned}\right\} \tag{70}$$

$$\left.\begin{aligned}
\mathsf{f}_{01}^{(1)}(\mathcal{E}) &= \nu_0'^2 - \mu_2(\mathcal{E}-\mu_0), \\
\mathsf{f}_{02}^{(1)}(\mathcal{E}) &= (\nu_1 - \nu)(\mathcal{E}-\mu_0) + \nu_0\nu_0', \qquad \mathsf{f}_{03}^{(1)}(\mathcal{E}) = -(\mathcal{E}-\mu_0), \\
\mathsf{f}_{12}^{(1)}(\mathcal{E}) &= \nu_1(\nu_1 - \nu)(\mathcal{E}-\mu_0) - \nu_0(\nu_0\mu_2 - 2\nu_1\nu_0' + \nu\nu_0'), \\
\mathsf{f}_{13}^{(1)}(\mathcal{E}) &= -\nu_1(\mathcal{E}-\mu_0) - \nu_0\nu_0', \qquad \mathsf{f}_{23}^{(1)}(\mathcal{E}) = -\nu_0^2,
\end{aligned}\right\} \tag{71}$$

$$\left.\begin{aligned}
\mathsf{g}_{01}^{(0)}(\mathcal{E}) &= \mu_2, \qquad \mathsf{g}_{02}^{(0)}(\mathcal{E}) = \nu_1 - \nu, \qquad \mathsf{g}_{03}^{(0)}(\mathcal{E}) = -1, \\
\mathsf{g}_{12}^{(0)}(\mathcal{E}) &= \mu_2(\mathcal{E}-\mu_1) + \nu_1(\nu_1 - \nu), \\
\mathsf{g}_{13}^{(0)}(\mathcal{E}) &= -\nu_1, \qquad \mathsf{g}_{23}^{(0)}(\mathcal{E}) = \mathcal{E} - \mu_1,
\end{aligned}\right\} \tag{72}$$

$$\left.\begin{aligned}
\mathsf{g}_{01}^{(1)}(\mathcal{E}) &= 0, \qquad \mathsf{g}_{02}^{(1)}(\mathcal{E}) = 0, \qquad \mathsf{g}_{03}^{(1)}(\mathcal{E}) = 0, \\
\mathsf{g}_{12}^{(1)}(\mathcal{E}) &= \mu_2(\mathcal{E}-\mu_0) + \nu_0'^2, \\
\mathsf{g}_{13}^{(1)}(\mathcal{E}) &= 0, \qquad \mathsf{g}_{23}^{(1)}(\mathcal{E}) = \mathcal{E} - \mu_0,
\end{aligned}\right\} \tag{73}$$

Two-magnon excitation spectra for the cases (a) $S = 1/2$, $\beta = 0$, $\gamma = 3/4$, and (b) $S = 1$, $\beta = 0$, $\gamma = 1/2$ are given in Cyr *et al.* [12] Figures 1 and 2 respectively. The

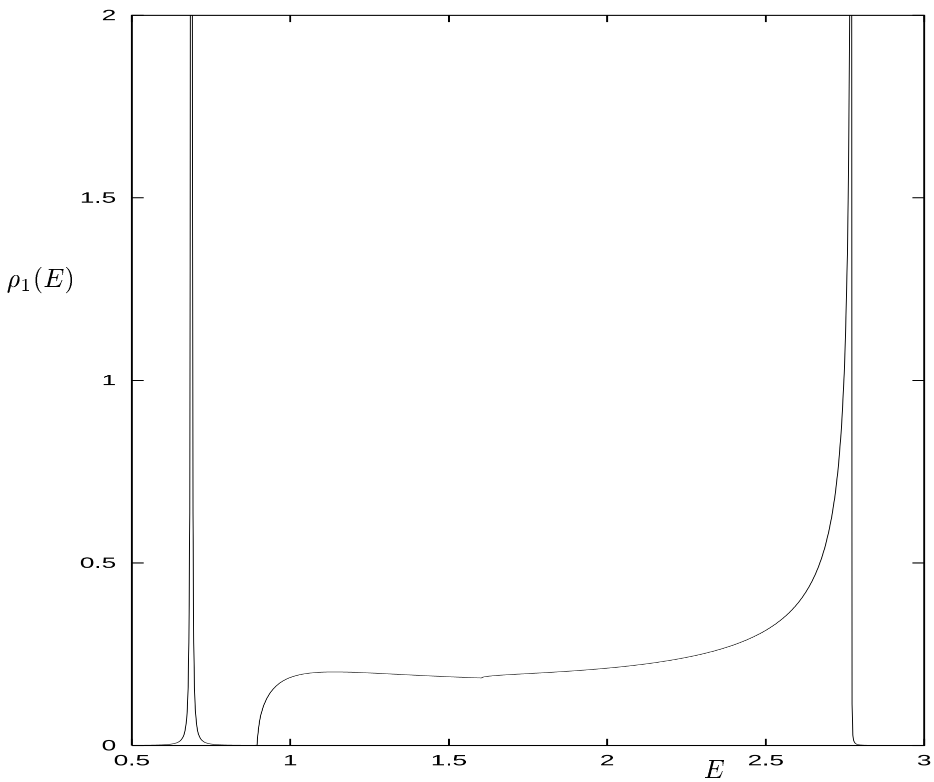

Figure 1: The density of states $\rho_1(E)$ for the case $S = 1/2$, $\beta = 0$, $\gamma = 3/4$, $K = \pi/2$. The energy is measured in units of $2SJ_1$.

lower and upper band edges of the scattering state continuum are given respectively by the least and greatest of the three quantities

$$E_b^{(\pm)} = \varepsilon + 2(V' \pm V), \qquad\qquad E_t = \varepsilon - 2V' - \frac{V^2}{4V'}. \tag{74}$$

This gives continuum band-edges in units of $E/2SJ_1$ for the two cases as (a) 0.8964 and 2.7708, and (b) 0.7929 and 2.6250 respectively. In case (a) the condition $S = 1/2$ gives from equations (67) and (70) $\mathsf{F}^{(0)}(\mathcal{E}) = 0$ and thus $G_0(E) = 1/(E - \varepsilon_0)$. In terms of the matrix calculation the leading row and column of $\mathbf{A}$ contains only zeros apart from $a(0,0) = (\varepsilon - E)/V'$ giving $G_0(E) = -\{(a(0,0)V'\}^{-1}$. In the two-magnon picture $\rho_0(E)$ is the density of the scattering state continuum for two magnons (spin deviations) on the same site. This is, of course, impossible for $S = 1/2$. In Figure 1 the density of states, $\rho_1(E)$, for two magnons on neighbouring sites is shown for the case $S = 1/2$, $\beta = 0$, $\gamma = 3/4$ $K = \pi/2$. The narrow peak below the broad continuum region is a bound state. If the energy is taken to be purely real this becomes a delta function as does also the singularity at the upper end of the continuum. To broaden these regions to make them more easily seen the energy was given an imaginary part of 10^{-4}i. In Figure 2 $\rho_0(E)$ is shown for the case $S = 1$, $\beta = 0$, $\gamma = 1/2$ $K = \pi/2$. For $S = 1$ this is a physical situation where two spin deviations can exist on the same site. Again the bound state delta function below the continuum is broadened into a lorenzian by using an imaginary part 10^{-4}i in the energy. This also has the effect of softening the step-function decrease to zero at the upper end of the continuum.

5 Conclusions

In this paper we extend the work of Lavis and Southern [7] to the case of semi-infinite symmetric banded matrices, which are Toeplitz for all but a finite number

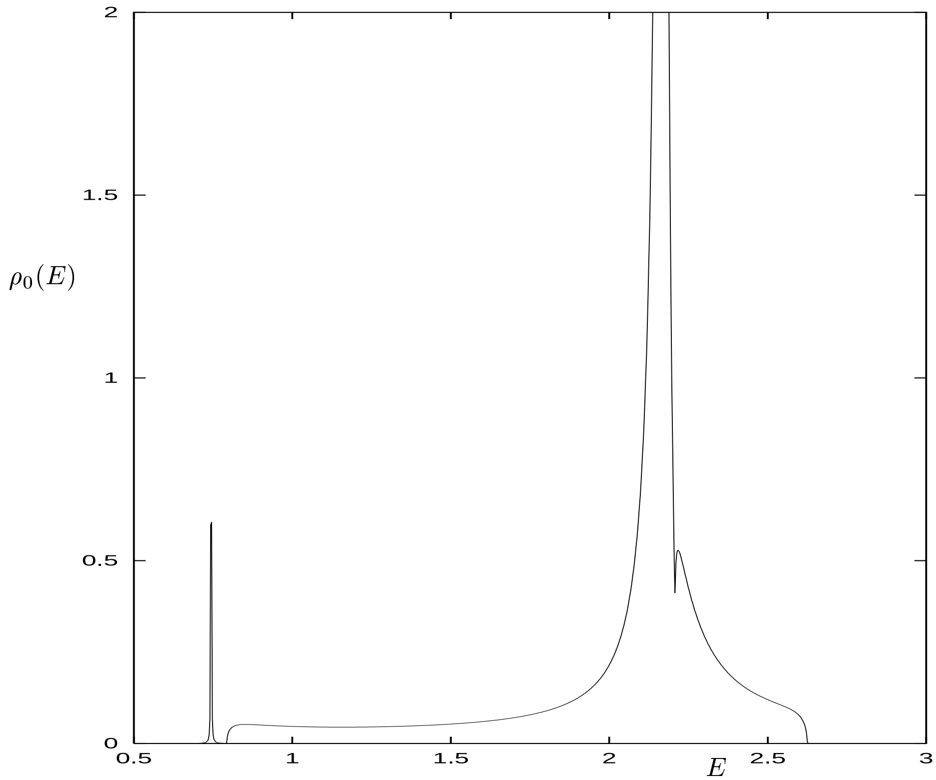

Figure 2: The density of states $\rho_0(E)$ for the case $S = 1$, $\beta = 0$, $\gamma = 1/2$, $K = \pi/2$. The energy is measured in units of $2SJ_1$.

of elements. As in [7] the only explicit matrix inversion that is required in of an $n \times n$ matrix when the bandwidth is $2n + 1$. Our procedure provides the analytic details required for the two-magnon calculations presented by Cyr, Southern and Lavis [12]. The method will also provide a straightforward procedure which can be used in a range of physical problems for which inversion of this type of matrix is required.

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