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The inverse of a semi-infinite symmetric banded matrix

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Abstract. We describe a method for obtaining an analytic form for an inverse of 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 $\mathbf{A}$ 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 eigenvalues and eigenvectors 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 generalized to matrices of bandwidth greater than three by Simons [6] and to symmetric tridiagonal matrices without the Toeplitz property by Yamani and Abdelmonem [7]. Results similar to those of Simons have been obtained by Lavis and Southern [8] using a transfer matrix rescaling method which has been utilized for excitations in tight-binding systems [9, 10] and quantum spin chains [11–13]. 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. An important difference between finite non-singular square matrices and semi-infinite (or infinite) matrices is that whereas the former have unique inverses the latter may have an infinite number of inverses. This situation occurs because of the possible existence of a non-trivial matrix $\mathbf{C}$ which is for $\mathbf{A}$ a divisor of zero; $\mathbf{AC} = \mathbf{0}$. Then if $\mathbf{B}$ is an inverse of $\mathbf{A}$ all matrices of the form $\mathbf{B} + \lambda\mathbf{C}$ will also be inverses. As will be seen the *existence* of divisors of zero plays a crucial role in our method. However, only one inverse is generated by the procedure with the associated divisor of zero being *identically* zero. There is, therefore, no ambiguity when the procedure is applied to physical problems.

We consider the semi-infinite symmetric banded matrices $\mathbf{A}$ of the form†

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

† For any matrix $\mathbf{X}$ we denote the row and column vectors formed by its ℓth row and jth column by $\langle\ell|\mathbf{X}$ and $\mathbf{X}|j\rangle$ respectively and the ℓ, jth element by $\langle\ell|\mathbf{X}|j\rangle$.

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where $a(\ell, \ell+n) \neq 0$ for $\ell = 0, 1, \ldots$. The Toeplitz property is taken to apply to all elements except those lying in the leading $(\tau+1) \times (\tau+1)$ submatrix. Thus

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

Without loss of generality let $\alpha(n) = 1$. It can be shown that matrices of this type are bounded operators on the class of square-summable semi-infinite vectors.

In section 2 we derive the general form for an inverse of A. In section 3 explicit results are given for tridiagonal ($n = 1$) and pentadiagonal ($n = 2$) cases. The first of these can be used to rederive the results of Lavis *et al* [14] for a semi-infinite tight-binding system with a surface adatom and an impurity located in the bulk. In section 4 the results for the pentadiagonal case are used to obtain the two-magnon spectrum of a generalized spin-S Heisenberg chain and our conclusions are presented in section 5.

2. Method

Given that B is an 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 $\ell, j \geqslant 0$ 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

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

and the $2n \times 2n$ matrices

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

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

Then equation (3) can be expressed in the form

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

Iterating (7) gives

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

where

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

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

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

where

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

The problem now is to obtain an expression for the elements of powers of the matrix $\mathbf{T}$. In a previous paper [8] two of the authors have shown that this can be done by defining

$$X_q(x) = \sum_{r=0}^{2n-q} \alpha(|n-r|)x^{r+q} \qquad q = 0, 1, \ldots, 2n. \tag{12}$$

It is then not difficult to show that the eigenvalues of $\mathbf{T}$ are the roots x_k, x_k^{-1}, $k = 1, \ldots, n$ of

$$X_0(x) = 0 \tag{13}$$

with corresponding orthonormal left and right eigenvectors

$$\boldsymbol{X}(x) = \begin{pmatrix} X_1(x) \\ X_2(x) \\ \vdots \\ X_{2n}(x) \end{pmatrix} \qquad \boldsymbol{Y}(x) = \begin{pmatrix} Y_1(x) \\ Y_2(x) \\ \vdots \\ Y_{2n}(x) \end{pmatrix} \tag{14}$$

where

$$Y_p(x) = -\frac{x^{-p-1}}{X_0'(x)}. \tag{15}$$

Thus

$$\langle p|\mathbf{T}^m|q\rangle = \sum_{k=1}^{n}\{Y_p(x_k)X_q(x_k)x_k^m + Y_p(x_k^{-1})X_q(x_k^{-1})x_k^{-m}\}. \tag{16}$$

Setting $x_k = \exp(\mathrm{i}\theta_k)$ then gives

$$\langle p|\mathbf{T}^m|q\rangle = u_q(m-p+1) \qquad p, q = 1, \ldots, 2n \tag{17}$$

where

$$u_q(\mu) = \sum_{r=0}^{2n-q} \alpha(|n-q-r|) \sum_{k=1}^{n} \frac{\sin\{(n+\mu-r-1)\theta_k\}}{F'(\theta_k)} \tag{18}$$

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

$$0 = F(\theta) \equiv \cos(n\theta) + \tfrac{1}{2}\alpha(0) + \sum_{r=1}^{n-1} \alpha(r)\cos(r\theta) \tag{19}$$

with

$$u_q(\mu) = \begin{cases} -u_1(\mu-1) & \text{for } q = 2n \\ -\alpha(|n-q|)u_1(\mu-1) + u_{q+1}(\mu-1) & \text{for } 1 \leqslant q < 2n \end{cases} \tag{20}$$

$$u_1(\mu) = -u_{2n}(\mu+1) = -\sum_{k=1}^{n} \frac{\sin\{(n+\mu)\theta_k\}}{F'(\theta_k)}. \tag{21}$$

Then, from (10) and (17),

$$\langle p|\mathbf{\Phi}(\ell, m)|q\rangle = \begin{cases} \displaystyle\sum_{r=1}^{2n} u_r(\tau - p - \ell + 1)\langle r|\mathbf{\Phi}(\tau, m)|q\rangle & \ell > \tau \geqslant m \\ u_q(m - p - \ell), & \ell \geqslant m > \tau. \end{cases} \tag{22}$$

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

$$b(\ell, j) = \sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\ell, 0)|n+m\rangle b(m-1, j) - \frac{\langle n|\mathbf{\Phi}(\ell, j)|1\rangle}{a(j, j+n)}. \tag{23}$$

Thus all the elements in the jth 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 (23) by $\kappa\sigma$ for some positive integer σ and $\kappa = 1, 2, \ldots, n$ yields the set of equations

$$b(\kappa\sigma, j) = \sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\kappa\sigma, 0)|n+m\rangle b(m-1, j) - \frac{\langle n|\mathbf{\Phi}(\kappa\sigma, j)|1\rangle}{a(j, j+n)} \qquad \kappa = 1, 2, \ldots, n. \tag{24}$$

Let the $n \times n$ matrix

$$\mathbf{U}_\sigma = \begin{pmatrix} \langle n|\mathbf{\Phi}(\sigma, 0)|n+1\rangle & \langle n|\mathbf{\Phi}(\sigma, 0)|n+2\rangle & \cdots & \langle n|\mathbf{\Phi}(\sigma, 0)|2n\rangle \\ \langle n|\mathbf{\Phi}(2\sigma, 0)|n+1\rangle & \langle n|\mathbf{\Phi}(2\sigma, 0)|n+2\rangle & \cdots & \langle n|\mathbf{\Phi}(2\sigma, 0)|2n\rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle n|\mathbf{\Phi}(n\sigma, 0)|n+1\rangle & \langle n|\mathbf{\Phi}(n\sigma, 0)|n+2\rangle & \cdots & \langle n|\mathbf{\Phi}(n\sigma, 0)|2n\rangle \end{pmatrix}. \tag{25}$$

Then, by solving equations (23) for $b(\ell, j)$, $\ell = 0, 1, \ldots, n-1$ and substituting into (24),

$$b(\ell, j) = C_\sigma(\ell, j) + B_\sigma(\ell, j) \tag{26}$$

where

$$C_\sigma(\ell, j) = \sum_{\kappa=1}^{n}\sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\ell, 0)|n+m\rangle \langle m|\mathbf{U}_\sigma^{-1}|\kappa\rangle b(\kappa\sigma, j) \tag{27}$$

$$B_\sigma(\ell, j) = \frac{1}{a(j, j+n)} \left\{ \sum_{\kappa=1}^{n}\sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\ell, 0)|n+m\rangle \right.$$
$$\left. \times \langle m|\mathbf{U}_\sigma^{-1}|\kappa\rangle \langle n|\mathbf{\Phi}(\kappa\sigma, j)|1\rangle - \langle n|\mathbf{\Phi}(\ell, j)|1\rangle \right\}. \tag{28}$$

Now consider the limit $\sigma \to \infty$. In all the applications we consider in this paper the matrix $\mathbf{A} = E\,\mathbf{I} - \mathbf{H}$, where $\mathbf{H}$ is a Hamiltonian and E is the energy. The inverse is then a Green's function and a small positive imaginary part is needed in the energy [15] to impose the correct boundary conditions and determine the Green's function uniquely in the limit

$\sigma \to \infty$. The small imaginary part in $\alpha(0)$ will lead to imaginary parts in θ_k. Since the form for $u_q(\mu)$ given by (18) is invariant under the change of sign of the solutions $\theta_1, \ldots, \theta_n$ of (19) we can assume that the imaginary part of each θ_k is positive. Then

$$\begin{aligned} u_q(\mu - \kappa\sigma) &\simeq \sum_{r=0}^{2n-q} \alpha(|n-q-r|) \sum_{k=1}^{n} \frac{\exp\{(n+\mu-\kappa\sigma-r-1)\mathrm{i}\theta_k\}}{2\mathrm{i}F'(\theta_k)} \\ &\sim \exp\Big\{\kappa\sigma \max_k[\mathrm{Im}(\theta_k)]\Big\}. \end{aligned} \tag{29}$$

which, from (22) and (25), gives

$$\begin{aligned} \langle n|\mathbf{\Phi}(\kappa\sigma, j)|1\rangle &\sim \exp\Big\{\kappa\sigma \max_k[\mathrm{Im}(\theta_k)]\Big\} \\ \langle \ell+1|\mathbf{U}_\sigma^{-1}|\kappa\rangle &\sim \exp\Big\{-\kappa\sigma \max_k[\mathrm{Im}(\theta_k)]\Big\}. \end{aligned} \tag{30}$$

Using these formulae it is not difficult to see that, in the limit $\sigma \to \infty$, the matrix with elements

$$c(\ell, j) = \lim_{\sigma\to\infty} C_\sigma(\ell, j) \tag{31}$$

is a divisor of zero for $\mathbf{A}$ when *any* possible inverse with elements $b(\ell, j)$ in used. Thus, from (28), we have the formula

$$b(\ell, j) = \lim_{\sigma\to\infty} B_\sigma(\ell, j) = \frac{1}{a(j, j+n)} \left\{ \sum_{m=1}^{n} \langle n|\mathbf{\Phi}(\ell, 0)|n+m\rangle \Omega(m, j) - \langle n|\mathbf{\Phi}(\ell, j)|1\rangle \right\} \tag{32}$$

for the elements of an inverse $\mathbf{B}$ of $\mathbf{A}$, where

$$\Omega(m, j) = \lim_{\sigma\to\infty} \sum_{\kappa=1}^{n} \langle m|\mathbf{U}_\sigma^{-1}|\kappa\rangle\langle n|\mathbf{\Phi}(\kappa\sigma, j)|1\rangle. \tag{33}$$

It may appear to be the case that we can now generate a divisior of zero with elements $c(\ell, j)$ by substituting from (32) into (27) and (31); this in turn leads to a succession of further inverses and divisors of zero. However, with this particular form for $b(\ell, j)$, this situation does not arise since it is easy to verify that $c(\ell, j) = 0$ for all $\ell, j = 1, \ldots, n$.

3. Explicit formulae

3.1. The case $n = 1$

For $n = 1$, $\mathbf{U}_\sigma$ is a 1×1 matrix with $\langle 1|\mathbf{U}_\sigma|1\rangle = \{\langle 1|\mathbf{\Phi}(\sigma, 0)|2\rangle\}^{-1}$. From (32) and (33)

$$b(\ell, j) = \frac{1}{a(j, j+1)} \{\langle 1|\mathbf{\Phi}(\ell, 0)|2\rangle \Omega(1, j) - \langle 1|\mathbf{\Phi}(\ell, j)|1\rangle\} \tag{34}$$

where

$$\Omega(1, j) = \lim_{\sigma\to\infty} \frac{\langle 1|\mathbf{\Phi}(\sigma, j)|1\rangle}{\langle 1|\mathbf{\Phi}(\sigma, 0)|2\rangle}. \tag{35}$$

From (21),

$$u_1(\mu) = -u_2(\mu+1) = \mathfrak{U}_\mu(\cos(\theta)) \qquad 2\cos(\theta) = -\alpha(0) \tag{36}$$

where

$$\mathfrak{U}_\mu(\cos(\theta)) = \frac{\sin\{(\mu+1)\theta\}}{\sin(\theta)} \tag{37}$$

is the Chebyshev polynomial of the second kind and, from (22),

$$\langle 1|\mathbf{\Phi}(\ell,m)|q\rangle = \begin{cases} \dfrac{\sin\{(\tau-\ell+1)\theta\}\langle 1|\mathbf{\Phi}(\tau,m)|q\rangle - \sin\{(\tau-\ell)\theta\}\langle 2|\mathbf{\Phi}(\tau,m)|q\rangle}{\sin(\theta)} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \ell > \tau \geqslant m,\ q=1,2 \\ \dfrac{\sin\{(m-\ell)\theta\}}{\sin(\theta)} \qquad\qquad\qquad\qquad \ell \geqslant m > \tau,\ q=1 \\ -\dfrac{\sin\{(m-\ell-1)\theta\}}{\sin(\theta)} \qquad\qquad\qquad \ell \geqslant m > \tau,\ q=2. \end{cases} \tag{38}$$

For simplicity we consider the case $\tau = 0$. $\mathbf{A}$ is a tridiagonal semi-infinite Toeplitz matrix with $a(\ell,\ell\pm 1) = 1$, $a(\ell,\ell) = \alpha(0)$, except for the leading diagonal element $a(0,0) \neq \alpha(0)$. From (5) and (9)

$$\mathbf{\Phi}(0,0) = \mathbf{T}_0^{-1} = \begin{pmatrix} 0 & 1 \\ -1 & -a(0,0) \end{pmatrix} \tag{39}$$

and, from (32), (34) and (38),

$$b(\ell,j) = f(\ell,j) + \mathrm{i}g(i,j) \tag{40}$$

where

$$f(\ell,j) = \begin{cases} f_1(\ell,j) & \ell \leqslant j \\ f_1(j,\ell) & \ell > j \end{cases} \tag{41}$$

and

$$\begin{aligned} f_1(\ell,j) &= -\frac{[\sin\{\ell\theta\}a(0,0) + \sin\{(\ell-1)\theta\}][\cos\{j\theta\}a(0,0) + \cos\{(j-1)\theta\}]}{\sin(\theta)\{1 + 2a(0,0)\cos(\theta) + [a(0,0)]^2\}} \\ g(\ell,j) &= -\frac{[\sin\{\ell\theta\}a(0,0) + \sin\{(\ell-1)\theta\}][\sin\{j\theta\}a(0,0) + \sin\{(j-1)\theta\}]}{\sin(\theta)\{1 + 2a(0,0)\cos(\theta) + [a(0,0)]^2\}}. \end{aligned} \tag{42}$$

From (26) and (31)

$$c(\ell,j) = \lim_{\sigma\to\infty} \frac{\langle 1|\mathbf{\Phi}(\ell,0)|2\rangle}{\langle 1|\mathbf{\Phi}(\sigma,0)|2\rangle} b(\sigma,j) \tag{43}$$

and it is not difficult to verify that with the form for the inverse given by (40) $c(\ell,j) = 0$. However, since the elements of $\mathbf{A}$ are real when $|\alpha(0)| \leqslant 2$, the matrix formed from the imaginary part $g(\ell,j)$ of the elements is a divisor of zero and the real part $f(\ell,j)$ alone is an inverse. In fact we can see that

$$\lim_{\sigma\to\infty} \frac{\langle 1|\mathbf{\Phi}(\ell,0)|2\rangle}{\langle 1|\mathbf{\Phi}(\sigma,0)|2\rangle} f(\sigma,j) = \mathrm{i}g(\ell,j) \qquad \lim_{\sigma\to\infty} \frac{\langle 1|\mathbf{\Phi}(\ell,0)|2\rangle}{\langle 1|\mathbf{\Phi}(\sigma,0)|2\rangle} g(\sigma,j) = -g(\ell,j). \tag{44}$$

The *unique* divisor of zero derived by this process is $g(\ell,j)$ which for a semi-infinite version of the tight-binding chain considered by Lavis and Southern [8] will give the density of states.

In the $n = 1$ case (7) becomes a three-term recurrence relation for $b(\ell,j)$ which can be solved using continued fractions [16]. To use continued fractions when $n > 1$ the matrix would need first to be transformed into tridiagonal form.

3.2. The case $n = 2$

In this case $\mathbf{U}_\sigma$ is a 2×2 matrix and, from (28)

$$b(\ell, j) = \frac{1}{a(j, j+2)}\{\langle 2|\boldsymbol{\Phi}(\ell, 0)|3\rangle\Omega(1, j) - \langle 2|\boldsymbol{\Phi}(\ell, 0)|4\rangle\Omega(2, j) - \langle 2|\boldsymbol{\Phi}(\ell, j)|1\rangle\} \tag{45}$$

where

$$\Omega(m, j) = \lim_{\sigma\to\infty} \frac{\phi(2, 2; 2\sigma, \sigma; 5-m, 1; j)}{\phi(2, 2; 2\sigma, \sigma; 4, 3, 0)} \tag{46}$$

and

$$\phi(\ell, m; x, y; p, q; j) = \langle\ell|\boldsymbol{\Phi}(x, 0)|p\rangle\langle m|\boldsymbol{\Phi}(y, j)|q\rangle - \langle m|\boldsymbol{\Phi}(y, 0)|p\rangle\langle\ell|\boldsymbol{\Phi}(x, j)|q\rangle. \tag{47}$$

Equation (19) is now a quadratic in the variable $\mathfrak{z} = \cos(\theta)$ with roots $\mathfrak{z}^{(+)}$ and $\mathfrak{z}^{(-)}$ given by

$$\mathfrak{z}^{(\pm)} = \mathfrak{z}(\pm\mathcal{Z}) = \tfrac{1}{4}\{-\alpha(1) \pm \mathcal{Z}\} \tag{48}$$

where

$$\mathcal{Z} = \sqrt{[\alpha(1)]^2 + 8 - 4\alpha(0)}. \tag{49}$$

We define

$$\mathfrak{V}(\ell) = \frac{\mathfrak{U}_\ell(\mathfrak{z}^{(+)}) - \mathfrak{U}_\ell(\mathfrak{z}^{(-)})}{2\{\mathfrak{z}^{(+)} - \mathfrak{z}^{(-)}\}} \tag{50}$$

where, from (37),

$$\mathfrak{V}(-\ell) = -\mathfrak{V}(\ell - 2) \tag{51}$$

and, from (19)–(21),

$$\left.\begin{aligned}
u_1(\ell) &= \mathfrak{V}(\ell+1)\\
u_2(\ell) &= -2\{1 + 2\mathfrak{z}^{(+)}\mathfrak{z}^{(-)}\}\mathfrak{V}(\ell) + 2\{\mathfrak{z}^{(+)} + \mathfrak{z}^{(-)}\}\mathfrak{V}(\ell-1) - \mathfrak{V}(\ell-2)\\
u_3(\ell) &= 2\{\mathfrak{z}^{(+)} + \mathfrak{z}^{(-)}\}\mathfrak{V}(\ell) - \mathfrak{V}(\ell-1)\\
u_4(\ell) &= -\mathfrak{V}(\ell).
\end{aligned}\right\} \tag{52}$$

Let

$$\begin{aligned}
\mathfrak{W}_\sigma(x, y) = {}& \mathfrak{V}(x + 2\sigma - \tau - 2)\mathfrak{V}(y + \sigma - \tau - 2)\\
& - \mathfrak{V}(x + \sigma - \tau - 2)\mathfrak{V}(y + 2\sigma - \tau - 2).
\end{aligned} \tag{53}$$

Then, from (22) and (47), when $\tau \geqslant j$,

$$\begin{aligned}
\phi(2, 2; 2\sigma, \sigma; p, q; j) = {}& \mathfrak{C}_{01}(p, q; j)\mathfrak{W}_\sigma(0, 1) + \mathfrak{C}_{02}(p, q; j)\mathfrak{W}_\sigma(0, 2)\\
& + \mathfrak{C}_{03}(p, q; j)\mathfrak{W}_\sigma(0, 3) + \mathfrak{C}_{12}(p, q; j)\mathfrak{W}_\sigma(1, 2)\\
& + \mathfrak{C}_{13}(p, q; j)\mathfrak{W}_\sigma(1, 3) + \mathfrak{C}_{23}(p, q; j)\mathfrak{W}_\sigma(2, 3)
\end{aligned} \tag{54}$$

where

$$\left.\begin{aligned}
\mathfrak{C}_{01}(p, q; j) = {}& -\alpha(0)\phi(1, 2; \tau, \tau; p, q; j) - \alpha(1)\phi(1, 3; \tau, \tau; p, q; j)\\
& - \phi(1, 4; \tau, \tau; p, q; j)\\
\mathfrak{C}_{02}(p, q; j) = {}& -\alpha(1)\phi(1, 2; \tau, \tau; p, q; j) - \phi(1, 3; \tau, \tau; p, q; j)\\
\mathfrak{C}_{03}(p, q; j) = {}& -\phi(1, 2; \tau, \tau; p, q; j)\\
\mathfrak{C}_{12}(p, q; j) = {}& (\alpha(0) - \alpha(1)^2)\phi(2, 3; \tau, \tau; p, q; j) - \alpha(1)\phi(2, 4; \tau, \tau; p, q; j)\\
& - \phi(3, 4; \tau, \tau; p, q; j)\\
\mathfrak{C}_{13}(p, q; j) = {}& -\alpha(1)\phi(2, 3; \tau, \tau; p, q; j) - \phi(2, 4; \tau, \tau; p, q; j)\\
\mathfrak{C}_{23}(p, q; j) = {}& -\phi(2, 3; \tau, \tau; p, q; j).
\end{aligned}\right\} \tag{55}$$

When $j > \tau$ the form of $\phi(2, 2; 2\sigma, \sigma; p, q; j)$ differs according to the value of q. However, from (45), we need only the cases $q = 1$ and $q = 3$ which are given by

$$\begin{aligned}\phi(2, 2; 2\sigma, \sigma; p, 1; j) = {} & \mathfrak{A}_{01}(p)\mathfrak{W}_\sigma(0, 1 + j - \tau) + \mathfrak{A}_{11}(p)\mathfrak{W}_\sigma(1, 1 + j - \tau) \\ & + \mathfrak{A}_{21}(p)\mathfrak{W}_\sigma(2, 1 + j - \tau) + \mathfrak{A}_{31}(p)\mathfrak{W}_\sigma(3, 1 + j - \tau)\end{aligned} \tag{56}$$

where

$$\left.\begin{aligned}\mathfrak{A}_{01}(p) &= \langle 1|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{A}_{11}(p) &= -\alpha(0)\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle - \alpha(1)\langle 3|\mathbf{\Phi}(\tau, 0)|p\rangle - \langle 4|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{A}_{21}(p) &= -\alpha(1)\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle - \langle 3|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{A}_{31}(p) &= \langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle\end{aligned}\right\} \tag{57}$$

and

$$\begin{aligned}\phi(2, 2; 2\sigma, \sigma; p, 3; j) = {} & \mathfrak{B}_{02}(p)\mathfrak{W}_\sigma(0, 2 + j - \tau) + \mathfrak{B}_{03}(p)\mathfrak{W}_\sigma(0, 3 + j - \tau) \\ & + \mathfrak{B}_{12}(p)\mathfrak{W}_\sigma(1, 2 + j - \tau) + \mathfrak{B}_{13}(p)\mathfrak{W}_\sigma(1, 3 + j - \tau) \\ & + \mathfrak{B}_{22}(p)\mathfrak{W}_\sigma(2, 2 + j - \tau) + \mathfrak{B}_{23}(p)\mathfrak{W}_\sigma(2, 3 + j - \tau) \\ & + \mathfrak{B}_{32}(p)\mathfrak{W}_\sigma(3, 2 + j - \tau) + \mathfrak{B}_{33}(p)\mathfrak{W}_\sigma(3, 3 + j - \tau)\end{aligned} \tag{58}$$

where

$$\left.\begin{aligned}\mathfrak{B}_{02}(p) &= -\alpha(1)\langle 1|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{03}(p) &= -\langle 1|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{12}(p) &= \alpha(0)\alpha(1)\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle + \alpha(1)^2\langle 3|\mathbf{\Phi}(\tau, 0)|p\rangle + \alpha(1)\langle 4|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{13}(p) &= \alpha(0)\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle + \alpha(1)\langle 3|\mathbf{\Phi}(\tau, 0)|p\rangle + \langle 4|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{22}(p) &= \alpha(1)^2\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle + \alpha(1)\langle 3|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{23}(p) &= \alpha(1)\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle + \langle 3|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{32}(p) &= \alpha(1)\langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle \\ \mathfrak{B}_{33}(p) &= \langle 2|\mathbf{\Phi}(\tau, 0)|p\rangle.\end{aligned}\right\} \tag{59}$$

It is not difficult to show that

$$\lim_{\sigma\to\infty} \frac{\mathfrak{W}_\sigma(x, y)}{\mathfrak{W}_\sigma(0, 1)} = \frac{[\zeta(\mathcal{Z})]^y[\zeta(-\mathcal{Z})]^x - [\zeta(\mathcal{Z})]^x[\zeta(-\mathcal{Z})]^y}{\zeta(\mathcal{Z}) - \zeta(-\mathcal{Z})} \tag{60}$$

where

$$\zeta(\pm\mathcal{Z}) = \mathcal{M}[\mathfrak{z}(\pm\mathcal{Z})] \tag{61}$$

and

$$\mathcal{M}[\mathfrak{z}] \equiv \text{the root of larger magnitude of } \{q^2 + 2\mathfrak{z}q + 1 = 0\}. \tag{62}$$

This enables $b(\ell, j)$ to be obtained from (45). The possibility of the roots in (62) being degenerate in magnitude is, as indicated above, removed by the introduction of a small imaginary part in $\alpha(0)$ and thus in $\mathfrak{z}(\pm\mathcal{Z})$.

4. Two-magnon excitations

The multi-magnon spectra of generalized spin-S Heisenberg chains with nearest-neighbour interactions have recently been studied using scaling [11] and recursion [12] 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* [13] applied the recursion method to obtain the three-magnon spectrum of the next-nearest-neighbour model with Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{i=1}^{N}\{J_1\tilde{S}_i \cdot \tilde{S}_{i+1} + J_2\tilde{S}_i \cdot \tilde{S}_{i+2} + J_3\tilde{S}_{i-1} \cdot (\tilde{S}_i \times \tilde{S}_{i+1})\} \tag{63}$$

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 (63) with energy $E_0 = -NS^2(J_1 + J_2)$. We shall study the excitation spectrum of (63) relative to the ferromagnetic state. The one-magnon excitation energy is given by

$$E_1 = 2S\{J_1 + 2SJ_3 \sin(ka_0)\}\{1 - \cos(ka_0)\} + 2SJ_2\{1 - \cos(2ka_0)\} \tag{64}$$

where k is a wavevector in the range $-\pi/a_0 \leqslant k \leqslant \pi/a_0$. Assuming that $J_1 > 0$ the condition that $E_1 \geqslant 0$ is that

$$\begin{aligned} &1 + 2\beta + \mathrm{sign}(\beta)\sqrt{4\beta^2 + \gamma^2} \geqslant 0 \qquad \text{if } \beta \neq 0 \\ &\gamma \leqslant 1 \qquad \text{if } \beta = 0 \end{aligned} \tag{65}$$

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

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 [17] considered the Hamiltonian in (63) with $J_3 = 0$ and $S = \frac{1}{2}$ and Bahurmuz and Loly [18] 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

$$|i, j\rangle = S_i^+ S_j^+ |0\rangle \qquad i \leqslant j \tag{66}$$

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 wavevector 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

$$\hat{\mathcal{H}} = \sum_{\ell=0}^{\infty}\{|K; \ell\rangle\varepsilon_\ell\langle K; \ell| + |K; \ell\rangle V_\ell\langle K; \ell + 1| + |K; \ell\rangle V'_\ell\langle K; \ell + 2|\} \tag{67}$$

where

$$\left.\begin{aligned}
&\varepsilon_0 = 4S(J_1 + J_2)\\
&\varepsilon_1 = (4S-1)J_1 + 2SJ_2\{2-\cos(K)\} + 2S(1-S)J_3\sin(K)\\
&\varepsilon_2 = 4SJ_1 + (4S-1)J_2\\
&\varepsilon_\ell = \varepsilon = 4SJ_1 + 4SJ_2 \qquad \ell \geqslant 3\\
&V_0 = -2\sqrt{S(2S-1)}J_1\cos(K/2) + 4SJ_3\sqrt{S(2S-1)}\sin(K/2)\\
&V_1 = -2SJ_1\cos(K/2) + 2S(2S-1)J_3\sin(K/2)\\
&V_\ell = V = -2SJ_1\cos(K/2) + 4S^2J_3\sin(K/2) \qquad \ell \geqslant 2\\
&V_0' = -2\sqrt{S(2S-1)}J_2\cos(K) - 2SJ_3\sqrt{S(2S-1)}\sin(K)\\
&V_\ell' = V' = -2SJ_2\cos(K) - 2S^2J_3\sin(K) \qquad \ell \geqslant 1.
\end{aligned}\right\} \tag{68}$$

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

$$\hat{\mathcal{G}}(E)\{E\hat{\mathcal{I}} - \hat{\mathcal{H}}\} = \hat{\mathcal{I}}. \tag{69}$$

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

$$\rho_\ell(E) = -\lim_{\delta\to 0+} \frac{\mathrm{Im}\{G_\ell(E+\mathrm{i}\delta)\}}{\pi}. \tag{70}$$

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_0. Comparing equations (1) and (2) with (67) and (68) we see that the matrix $\mathbf{A}$ with elements

$$a(\ell, j) = -\langle K;\ell|\frac{\{E\hat{\mathcal{I}} - \hat{\mathcal{H}}\}}{V'}|K;j\rangle \tag{71}$$

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

$$\left.\begin{aligned}
&a(\ell,\ell) = \begin{cases} \mu_\ell - \mathcal{E} & \ell \leqslant 2\\ \alpha(0) = -\mathcal{E} & \ell > 2\end{cases}\\
&a(\ell,\ell+1) = a(\ell+1,\ell) = \begin{cases} \nu_\ell & \ell \leqslant 1\\ \alpha(1) = \nu & \ell > 1\end{cases}\\
&a(\ell,\ell+2) = a(\ell+2,\ell) = \begin{cases} \nu_0' & \ell = 0\\ 1 & \ell > 0\end{cases}
\end{aligned}\right\} \tag{72}$$

where

$$\left.\begin{aligned}
&\mathcal{E} = \frac{E-\varepsilon}{V'} \qquad \mu_\ell = \frac{\varepsilon_\ell - \varepsilon}{V'} \qquad \ell = 0, 1, 2\\
&\nu = \frac{V}{V'} \qquad \nu_\ell = \frac{V_\ell}{V'} \qquad \ell = 0, 1 \qquad \nu_0' = \frac{V_0'}{V'}
\end{aligned}\right\} \tag{73}$$

and from (48)

$$\mathfrak{z}^{(\pm)} = \mathfrak{z}(\pm\mathcal{Z}(\mathcal{E})) = \tfrac{1}{4}\{-\nu \pm \mathcal{Z}(\mathcal{E})\} \tag{74}$$

with

$$\mathcal{Z}(\mathcal{E}) = \sqrt{\nu^2 + 8 + 4\mathcal{E}}. \tag{75}$$

With these definitions for the elements of **A** the matrix elements of the Green's function are given in terms of the inverse matrix **B** by

$$\langle K;\ell|\hat{\mathcal{G}}(\mathcal{E})|K;j\rangle = -\frac{b(\ell,j)}{V'}. \tag{76}$$

In particular the two leading diagonal Green's functions are

$$G_\ell(E) = \langle K;\ell|\hat{\mathcal{G}}(\mathcal{E})|K;\ell\rangle = \frac{1}{V'}\frac{\mathfrak{G}^{(\ell)}(\mathcal{E})}{(\mathcal{E}-\mu_\ell)\mathfrak{G}^{(\ell)}(\mathcal{E})+\mathfrak{F}^{(\ell)}(\mathcal{E})} \qquad \ell = 0,1 \tag{77}$$

where

$$\mathfrak{F}^{(\ell)}(\mathcal{E}) = \mathfrak{f}_{01}^{(\ell)}(\mathcal{E}) + \mathfrak{f}_{02}^{(\ell)}(\mathcal{E})A(\mathcal{E}) + \mathfrak{f}_{03}^{(\ell)}(\mathcal{E})\{[A(\mathcal{E})]^2 - B(\mathcal{E})\} + \mathfrak{f}_{12}^{(\ell)}(\mathcal{E})B(\mathcal{E}) + \mathfrak{f}_{13}^{(\ell)}(\mathcal{E})A(\mathcal{E})B(\mathcal{E}) + \mathfrak{f}_{23}^{(\ell)}(\mathcal{E})[B(\mathcal{E})]^2 \tag{78}$$

$$\mathfrak{G}^{(\ell)}(\mathcal{E}) = \mathfrak{g}_{01}^{(\ell)}(\mathcal{E}) + \mathfrak{g}_{02}^{(\ell)}(\mathcal{E})A(\mathcal{E}) + \mathfrak{g}_{03}^{(\ell)}(\mathcal{E})\{[A(\mathcal{E})]^2 - B(\mathcal{E})\} + \mathfrak{g}_{12}^{(\ell)}(\mathcal{E})B(\mathcal{E}) + \mathfrak{g}_{13}^{(\ell)}(\mathcal{E})A(\mathcal{E})B(\mathcal{E}) + \mathfrak{g}_{23}^{(\ell)}(\mathcal{E})[B(\mathcal{E})]^2 \tag{79}$$

$$\left.\begin{aligned} A(\mathcal{E}) &= \zeta(\mathcal{Z}(\mathcal{E})) + \zeta(-\mathcal{Z}(\mathcal{E})) \\ B(\mathcal{E}) &= \zeta(\mathcal{Z}(\mathcal{E}))\zeta(-\mathcal{Z}(\mathcal{E})) \end{aligned}\right\} \tag{80}$$

$$\left.\begin{aligned} &\mathfrak{f}_{01}^{(0)}(\mathcal{E}) = \nu_0'^2 \qquad \mathfrak{f}_{02}^{(0)}(\mathcal{E}) = \nu_0'\nu_0 \qquad \mathfrak{f}_{03}^{(0)}(\mathcal{E}) = 0 \\ &\mathfrak{f}_{12}^{(0)}(\mathcal{E}) = \nu_0'^2(\mathcal{E}-\mu_1) - \nu_0\nu_0'(\nu - 2\nu_1) - \nu_0^2\mu_2 \\ &\mathfrak{f}_{13}^{(0)}(\mathcal{E}) = -\nu_0\nu_0' \qquad \mathfrak{f}_{23}^{(0)}(\mathcal{E}) = -\nu_0^2 \end{aligned}\right\} \tag{81}$$

$$\left.\begin{aligned} &\mathfrak{f}_{01}^{(1)}(\mathcal{E}) = \nu_0'^2 - \mu_2(\mathcal{E}-\mu_0) \\ &\mathfrak{f}_{02}^{(1)}(\mathcal{E}) = (\nu_1-\nu)(\mathcal{E}-\mu_0) + \nu_0\nu_0' \qquad \mathfrak{f}_{03}^{(1)}(\mathcal{E}) = -(\mathcal{E}-\mu_0) \\ &\mathfrak{f}_{12}^{(1)}(\mathcal{E}) = \nu_1(\nu_1-\nu)(\mathcal{E}-\mu_0) - \nu_0(\nu_0\mu_2 - 2\nu_1\nu_0' + \nu\nu_0') \\ &\mathfrak{f}_{13}^{(1)}(\mathcal{E}) = -\nu_1(\mathcal{E}-\mu_0) - \nu_0\nu_0' \qquad \mathfrak{f}_{23}^{(1)}(\mathcal{E}) = -\nu_0^2 \end{aligned}\right\} \tag{82}$$

$$\left.\begin{aligned} &\mathfrak{g}_{01}^{(0)}(\mathcal{E}) = \mu_2 \qquad \mathfrak{g}_{02}^{(0)}(\mathcal{E}) = \nu_1 - \nu \qquad \mathfrak{g}_{03}^{(0)}(\mathcal{E}) = -1 \\ &\mathfrak{g}_{12}^{(0)}(\mathcal{E}) = \mu_2(\mathcal{E}-\mu_1) + \nu_1(\nu_1-\nu) \\ &\mathfrak{g}_{13}^{(0)}(\mathcal{E}) = -\nu_1 \qquad \mathfrak{g}_{23}^{(0)}(\mathcal{E}) = \mathcal{E} - \mu_1 \end{aligned}\right\} \tag{83}$$

$$\left.\begin{aligned} &\mathfrak{g}_{01}^{(1)}(\mathcal{E}) = 0 \qquad \mathfrak{g}_{02}^{(1)}(\mathcal{E}) = 0 \qquad \mathfrak{g}_{03}^{(1)}(\mathcal{E}) = 0 \\ &\mathfrak{g}_{12}^{(1)}(\mathcal{E}) = \mu_2(\mathcal{E}-\mu_0) + \nu_0'^2 \\ &\mathfrak{g}_{13}^{(1)}(\mathcal{E}) = 0 \qquad \mathfrak{g}_{23}^{(1)}(\mathcal{E}) = \mathcal{E} - \mu_0. \end{aligned}\right\} \tag{84}$$

Two-magnon excitation spectra for the cases (a) $S = \frac{1}{2}$, $\beta = 0$, $\gamma = \frac{3}{4}$, and (b) $S = 1$, $\beta = 0$, $\gamma = \frac{1}{2}$ are given in Cyr *et al* [13] and figures 1 and 2 respectively. The lower and upper band edges of the scattering state continuum are given, respectively, by the least and greatest of the three quantities

$$E_{\mathrm{b}}^{(\pm)} = \varepsilon + 2(V' \pm V) \qquad E_{\mathrm{t}} = \varepsilon - 2V' - \frac{V^2}{4V'}. \tag{85}$$

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 $S = \frac{1}{2}$ gives, from equations (78) and (81), $\mathfrak{F}^{(0)}(\mathcal{E}) = 0$ and thus $G_0(E) = 1/(E - \varepsilon_0)$. In terms of the matrix calculation the leading row and column of **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 $\rho_0(E)$

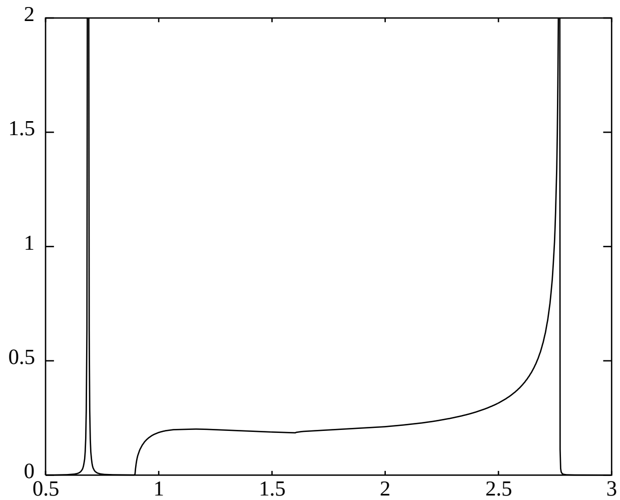

Figure 1. The density of states $\rho_1(E)$ for the case $S = \frac{1}{2}$, $\beta = 0$, $\gamma = \frac{3}{4}$, $K = \frac{\pi}{2}$. The energy is measured in units of $2SJ_1$.

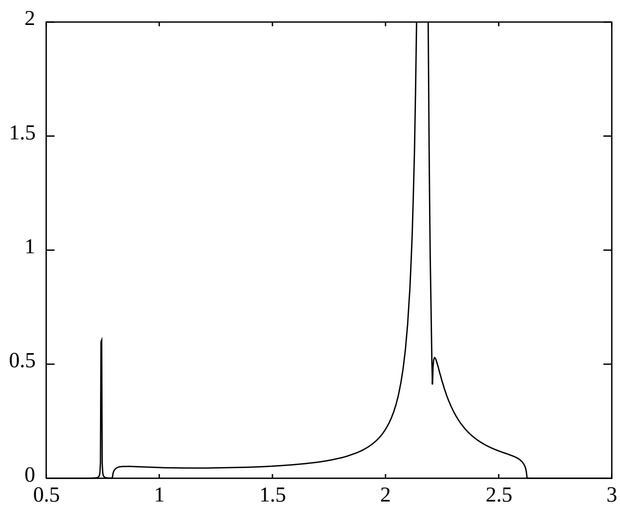

Figure 2. The density of states $\rho_0(E)$ for the case $S = 1$, $\beta = 0$, $\gamma = \frac{1}{2}$, $K = \frac{\pi}{2}$. The energy is measured in units of $2SJ_1$.

is the density of the scattering state continuum for two magnons (spin deviations) on the same site. This is, of course, impossible for $S = \frac{1}{2}$. In figure 1 the density of states, $\rho_1(E)$, for two magnons on neighbouring sites is shown for the case $S = \frac{1}{2}$, $\beta = 0$, $\gamma = \frac{3}{4}$, $K = \frac{\pi}{2}$. 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 $S = 1$, $\beta = 0$, $\gamma = \frac{1}{2}$, $K = \frac{\pi}{2}$. 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 have extended the work of Lavis and Southern [8] to the case of semi-infinite symmetric banded matrices which are Toeplitz for all but a finite number of elements. As in [8] the only explicit matrix inversion needed, when the bandwidth is $2n + 1$, is of an $n \times n$ matrix . Our procedure provides the analytic details for the two-magnon calculations presented by Cyr *et al* [13]. 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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References

[1] Calderón A, Spitzer F and Widom H 1959 *Ill. J. Math.* **3** 490
[2] Widom H 1960 *Ill. J. Math.* **4** 88
[3] Golub G H and Van Loan C F 1989 *Matrix Computations* (Baltimore, MD: Johns Hopkins University Press)
[4] Streater R F 1979 *Bull. London Math. Soc.* **11** 354
[5] Hu G Y and O'Connell R F 1996 *J. Phys. A: Math. Gen.* **29** 1511
[6] Simons S 1997 *J. Phys. A: Math. Gen.* **30** 755
[7] Yamani H A and Abdelmonem M S 1997 *J. Phys. A: Math. Gen.* **30** 2889
[8] Lavis D A and Southern B W 1997 *Rep. Math. Phys.* **39**, 137
[9] Southern B W, Kumar A A, Loly P D and Tremblay A-M S 1983 *Phys. Rev.* B **27** 1405
[10] Southern B W, Kumar A A and Ashraff J A 1983 *Phys. Rev.* B **28** 1785
[11] Southern B W, Liu T S and Lavis D A 1989 *Phys. Rev.* B **39** 160
[12] Southern B W, Lee R J and Lavis D A 1994 *J. Phys.: Condens. Matter* **6** 10 075
[13] Cyr S L M, Southern B W and Lavis D A 1996 *J. Phys.: Condens. Matter* **8** 4781
[14] Lavis D A, Southern B W and Davison S G 1985 *J. Phys. C: Solid State Phys.* **18** 1387
[15] Economou E N 1983 *Green's Functions in Quantum Physics (Springer Series in Solid-State Sciences 7)* (New York: Springer)
[16] Mathews J and Walker R L 1970 *Mathematical Methods of Physics* 2nd edn (New York: Benjamin)
[17] Majumdar C K 1969 *J. Math. Phys.* **10** 177
[18] Bahurmuz A A and Loly P D 1986 *J. Phys. C: Solid State Phys.* **19** 2241