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THE INVERSE OF A SYMMETRIC BANDED TOEPLITZ MATRIX

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We describe a method for obtaining an analytic form for the inverse of a finite symmetric banded Toeplitz matrix. Explicit formulae are given for the tridiagonal and pentadiagonal cases and the results are applied to the evaluation of the Green's function for nearest and next-nearest neighbour one-dimensional tight-binding systems.

1. Introduction

A Toeplitz matrix $\mathbf{A}$ has elements $A_{s,j}$ with the property $A_{s,j} = a(s-j)$. In the case of semi-infinite matrices $(s, j = 0, 1, \ldots)$ 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 by Hu and O'Connell [5] from a calculation of the determinant and cofactors of the matrix. The inverse of the symmetric tridiagonal matrix can be used in the solution of various single-charge-tunnelling problems and of the one-dimensional Poisson equation with Dirichlet boundary conditions. It also provides the Green's function for a one-dimensional homogeneous nearest-neighbour tight-binding system with open boundaries [6].

The rescaling method for excitations in tight-binding systems [7, 8] and quantum spin chains [9, 10] uses a transfer matrix approach. This has the potential to provide a generalization of Hu and O'Connell's result to all $N \times N$ matrices $\mathbf{A}$, with elements[1]

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

of the form

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

In Sections 2 and 3 we describe this procedure and give explicit formulae for band-widths $2n+1=3$ and $2n+1=5$. In Section 4 these results are applied to first and second neighbour tight-binding models on a finite one-dimensional lattice.

2. Method

Given that $\mathbf{B}$ is the inverse of $\mathbf{A}$,

$$\sum_{k=\alpha(s)}^{\beta(s)} a(|k|)\langle s+k|\mathbf{B}|j\rangle = \delta_{sj}, \tag{2}$$

where

$$\alpha(s) = \mathrm{Max}\{1-s,-n\}, \qquad \beta(s) = \mathrm{Min}\{N-s,n\}. \tag{3}$$

We define

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

where $b(s,j) = \langle s|\mathbf{B}|j\rangle$ if $1 \le s,j \le N$ and zero otherwise, and the transfer matrix

$$\mathbf{T} = \begin{pmatrix} -a(n-1) & -a(n-2) & \cdots & -a(0) & \cdots & -a(n-1) & -1 \\ 1 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & 1 & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & 0 & \cdots & \cdots & \cdots & 1 & 0 \end{pmatrix}. \tag{5}$$

Then equation (2) can be expressed in the form

$$\mathbf{T}\mathbf{b}_s(j) = \mathbf{b}_{s-1}(j) - \delta_{s,j}\mathbf{I}|1\rangle. \tag{6}$$

Iterating (6) gives

$$\mathbf{b}_s(j) = \begin{cases} \mathbf{T}^{-s}\mathbf{b}_0(j), & \text{if } j > s, \\ \mathbf{T}^{-s}\mathbf{b}_0(j) - \mathbf{T}^{-(s-j+1)}|1\rangle & \text{if } j \le s. \end{cases} \tag{7}$$

The vector $\mathbf{b}_0(j)$ has zeros in the first n elements and so equation (7) gives

$$b(s,j) = \begin{cases} \sum_{k=1}^{n} \langle n|\mathbf{T}^{-s}|k+n\rangle b(k,j) & \text{if } j > s, \\ \sum_{k=1}^{n} \langle n|\mathbf{T}^{-s}|k+n\rangle b(k,j) - \langle n|\mathbf{T}^{-(s-j+1)}|1\rangle & \text{if } j \le s. \end{cases} \tag{8}$$

The vector $\mathbf{b}_N(j)$ has zeros in the last n elements, so, from (7),

$$0 = \sum_{k=1}^{n} \langle m+n|\mathbf{T}^{-N}|k+n\rangle b(k,j) - \langle m+n|\mathbf{T}^{-(N-j+1)}|1\rangle, \qquad m = 1,\ldots,n. \tag{9}$$

From equation (8) the N elements of the j-th column of $\mathbf{B}$ are given as as linear combinations of the first n elements which are in turn given as solutions of the n linear equations (9).

The remaining problem is to obtain an expression for the elements of powers of the transfer matrix $\mathbf{T}$. We define the functions

$$\phi_j(\mu) = \sum_{r=0}^{2n-j} a(|n-r|)\mu^{r+j}, \qquad j = 0,1,\ldots,2n. \tag{10}$$

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

$$\phi_0(\mu) = 0, \tag{11}$$

with corresponding orthonormal left and right eigenvectors

$$\boldsymbol{\phi}(\mu) = \begin{pmatrix} \phi_1(\mu) \\ \phi_2(\mu) \\ \vdots \\ \phi_{2n}(\mu) \end{pmatrix}, \qquad \boldsymbol{\psi}(\mu) = \begin{pmatrix} \psi_1(\mu) \\ \psi_2(\mu) \\ \vdots \\ \psi_{2n}(\mu) \end{pmatrix}, \tag{12}$$

where

$$\psi_s(\mu) = -\frac{\mu^{-s-1}}{\phi_0'(\mu)}. \tag{13}$$

Thus

$$\langle s|\mathbf{T}^m|j\rangle = \sum_{k=1}^{n} \{\psi_s(\mu_k)\phi_j(\mu_k)\mu_k^m + \psi_s(\mu_k^{-1})\phi_j(\mu_k^{-1})\mu_k^{-m}\}. \tag{14}$$

A more compact form is obtained by setting

$$\mu = \exp(\mathrm{i}\theta) \tag{15}$$

when we have

$$\langle s|\mathbf{T}^m|j\rangle = u_j(m-s+1), \qquad s,j = 1,\ldots,2n, \tag{16}$$

where, for $j = 1, \ldots, 2n$ and any integer ℓ,

$$u_j(\ell) = \sum_{r=0}^{2n-j} a(|n-j-r|) \sum_{k=1}^{n} \frac{\sin\{(n+\ell-r-1)\theta_k\}}{F'(\theta_k)} \tag{17}$$

and $\theta_1, \ldots, \theta_n$ are the roots of the equation

$$0 = F(\theta) \equiv \cos(n\theta) + \tfrac{1}{2}a(0) + \sum_{r=1}^{n-1} a(r)\cos(r\theta). \tag{18}$$

It follows from (4) and (14) that

$$u_j(\ell) = \begin{cases} -u_1(\ell-1) & \text{for } j = 2n, \\ -a(|n-j|)u_1(\ell-1) + u_{j+1}(\ell-1) & \text{for } 1 \le j < 2n. \end{cases} \tag{19}$$

Iterating the second of equations (19) and comparing with (17), we obtain the result

$$u_1(\ell) = -u_{2n}(\ell+1) = -\sum_{k=1}^{n} \frac{\sin\{(n+\ell)\theta_k\}}{F'(\theta_k)}. \tag{20}$$

We now define the set of $n \times n$ matrices

$$\mathbf{U}(\ell) = \begin{pmatrix} u_{n+1}(-\ell-n) & u_{n+2}(-\ell-n) & \cdots & u_{2n}(-\ell-n) \\ u_{n+1}(-\ell-n-1) & u_{n+2}(-\ell-n-1) & \cdots & u_{2n}(-\ell-n-1) \\ \vdots & \vdots & \vdots & \vdots \\ u_{n+1}(-\ell-2n+1) & u_{n+2}(-\ell-2n+1) & \cdots & u_{2n}(-\ell-2n+1) \end{pmatrix} \tag{21}$$

and, from (8), (9), (16) and (20),

$$b(s,j) = \begin{cases} -\langle 1|\mathbf{U}(s-1)[\mathbf{U}(N)]^{-1}\mathbf{U}(N-j)|n\rangle & \text{if } j > s, \\ -\langle 1|\left\{\mathbf{U}(s-1)[\mathbf{U}(N)]^{-1}\mathbf{U}(N-j) - \mathbf{U}(s-1-j)\right\}|n\rangle & \text{if } j \le s. \end{cases} \tag{22}$$

3. Explicit formulae

We use the procedure of the previous section to rederive the ($n = 1$) result of Hu and O'Connell [5] and to give the formula for the case $n = 2$.

3.1. The case $n = 1$

Now $\mathbf{U}(\ell)$ is a 1×1 matrix with

$$\mathbf{U}(\ell) = u_1(\ell) = -u_2(\ell+1) = \mathrm{U}_\ell(\cos\theta), \qquad 2\cos\theta = -a(0), \tag{23}$$

where

$$\mathrm{U}_\ell(\cos\theta) = \frac{\sin\{(\ell+1)\theta\}}{\sin\theta} \tag{24}$$

is the Chebyshev polynomial of the second kind. From (22) we obtain

$$b(s,j) = \frac{\cos\{(N+1-|s-j|)\theta\} - \cos\{(N+1-s-j)\theta\}}{2\sin\theta\sin\{(N+1)\theta\}}. \tag{25}$$

With the substitution

$$\theta = \begin{cases} \lambda & \text{if } |a(0)| < 2, \\ \mathrm{i}\lambda & \text{if } a(0) \le -2, \\ \mathrm{i}\lambda + \pi & \text{if } a(0) \ge 2, \end{cases} \tag{26}$$

for real λ, this is the result obtained by Hu and O'Connell [5].

3.2. The case $n = 2$

Let $\zeta_k = \cos\theta_k$, $k = 1, 2$. Then, from (18),

$$2(1 + 2\zeta_1\zeta_2) = a(0). \qquad 2(\zeta_1 + \zeta_2) = -a(1). \tag{27}$$

We define

$$\mathrm{V}(\ell) = \frac{\mathrm{U}_\ell(\zeta_1) - \mathrm{U}_\ell(\zeta_2)}{2(\zeta_1 - \zeta_2)} \tag{28}$$

and, from (24), (28) and (21), we get

$$\mathrm{V}(-\ell) = -\mathrm{V}(\ell - 2). \tag{29}$$

$$\mathbf{U}(\ell) = \begin{pmatrix} \mathrm{V}(\ell+1) - \mathrm{V}(2)\mathrm{V}(\ell) & \mathrm{V}(\ell) \\ \mathrm{V}(\ell+2) - \mathrm{V}(2)\mathrm{V}(\ell+1) & \mathrm{V}(\ell+1) \end{pmatrix}. \tag{30}$$

Substituting (30) into (22) it can be shown, after some manipulation, that

$$b(s,j) = \begin{cases} \dfrac{\mathrm{F}(s,j,N;\theta_1,\theta_2)}{\mathrm{F}(1,-1,N;\theta_1,\theta_2)} & \text{if } j \ge s, \\[2ex] \dfrac{\mathrm{F}(j,s,N;\theta_1,\theta_2)}{\mathrm{F}(1,-1,N;\theta_1,\theta_2)} & \text{if } j \le s, \end{cases} \tag{31}$$

where

$$\mathrm{F}(s,j,N;\theta_1,\theta_2) = \mathrm{V}(s-1)\mathrm{W}(N-j,N+1) - \mathrm{V}(s)\mathrm{W}(N-j,N) \tag{32}$$

and

$$\mathrm{W}(s,j) = \mathrm{V}(s+1)\mathrm{V}(j) - \mathrm{V}(s)\mathrm{V}(j+1). \tag{33}$$

From (24), (28) and (33) we obtain

$$\begin{aligned}
F(s,j,N;\theta_1,\theta_2) = {} & f_1(s-j,N;\theta_1,\theta_2) - f_1(s-j,N;\theta_2,\theta_1) + \\
& + g_1(s-j,N;\theta_1,\theta_2) - g_1(s-j,N;\theta_2,\theta_1) + \\
& + f_2(s+j,N;\theta_1,\theta_2) - f_2(s+j,N;\theta_2,\theta_1) + \\
& + g_2(s+j,N;\theta_1,\theta_2) - g_2(s+j,N;\theta_2,\theta_1) + \\
& + f_3(s,j,N;\theta_1,\theta_2) - f_3(s,j,N;\theta_2,\theta_1) + \\
& + g_3(s,j,N;\theta_1,\theta_2) - g_3(s,j,N;\theta_2,\theta_1) + \\
& + f_3(s,j,N;\theta_1,-\theta_2) - f_3(s,j,N;-\theta_2,\theta_1) + \\
& + g_3(s,j,N;\theta_1,-\theta_2) - g_3(s,j,N;-\theta_2,\theta_1),
\end{aligned} \tag{34}$$

where

$$\begin{aligned}
f_1(k,N;\theta_1,\theta_2) = {} & \sin(\theta_2)\cos(\theta_1 k)\{2\cos(2\theta_1+\theta_1 N)\sin(2\theta_2+\theta_2 N)- \\
& -\cos(3\theta_1+\theta_1 N)\sin(\theta_2+\theta_2 N)- \\
& -\cos(\theta_1+\theta_1 N)\sin(3\theta_2+\theta_2 N)\}, \\
g_1(k,N;\theta_1,\theta_2) = {} & \sin(\theta_2)\sin(\theta_1 k)\{2\sin(\theta_1)\sin(\theta_2)- \\
& -2\sin(2\theta_1+\theta_1 N)\sin(2\theta_2+\theta_2 N)+ \\
& +\sin(3\theta_1+\theta_1 N)\sin(\theta_2+\theta_2 N)+ \\
& +\sin(\theta_1+\theta_1 N)\sin(3\theta_2+\theta_2 N)\}, \\
f_2(k,N;\theta_1,\theta_2) = {} & 2\sin(\theta_2)\cos(\theta_1 k)\cos(\theta_1+\theta_1 N)\sin(2\theta_2+\theta_2 N)\times \\
& \times\{\cos(\theta_2)-\cos(\theta_1)\}, \\
g_2(k,N;\theta_1,\theta_2) = {} & 2\sin(\theta_2)\sin(\theta_1 k)\sin(\theta_1+\theta_1 N)\sin(2\theta_2+\theta_2 N)\times \\
& \times\{\cos(\theta_2)-\cos(\theta_1)\}, \\
f_3(s,j,N;\theta_1,\theta_2) = {} & \sin(\theta_1)\sin(\theta_2)\cos(\theta_1 s-\theta_2 j)\times \\
& \times\{\cos(\theta_2)-\cos(\theta_1)+ \\
& +\cos(\theta_1+\theta_1 N-2\theta_2-\theta_2 N)- \\
& -\cos(\theta_2+\theta_2 N-2\theta_1-\theta_1 N)\}, \\
g_3(s,j,N;\theta_1,\theta_2) = {} & \sin(\theta_1)\sin(\theta_2)\sin(\theta_1 s-\theta_2 j)\times \\
& \times\{\sin(\theta_2)+\sin(\theta_1)+ \\
& +\sin(\theta_1+\theta_1 N-2\theta_2-\theta_2 N)+ \\
& +\sin(\theta_2+\theta_2 N-2\theta_1-\theta_1 N)\}.
\end{aligned} \tag{35}$$

4. Tight-binding systems

The Hamiltonian of an n-th neighbour tight-binding system on a one-dimensional lattice of N sites is given by

$$\hat{H} = \sum_{s=1}^{N} \sum_{k=\alpha(s)}^{\beta(s)} |s\rangle \varepsilon_k \langle s+k|, \tag{36}$$

where $\alpha(s)$ and $\beta(s)$ are given by (3). The Green's function operator $\hat{G}(N;E)$ is defined, for energy E, by

$$\hat{G}(N;E)\{E\hat{I} - \hat{H}\} = \hat{I}. \tag{37}$$

Thus, with the identification,

$$a(0) = -2\gamma = \frac{\varepsilon_0 - E}{\varepsilon_n}, \qquad a(k) = \frac{\varepsilon_k}{\varepsilon_n}, \qquad k = 1,\ldots,n, \tag{38}$$

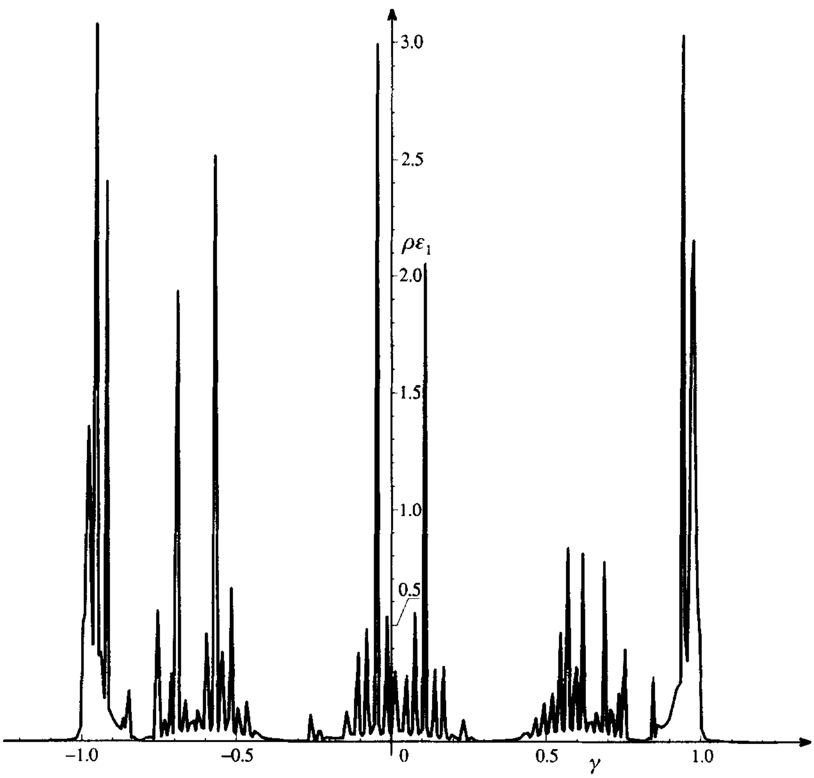

Fig. 1. Local density of states at site $s = 5$ plotted against γ for a one-dimensional nearest-neighbour tight-binding system of $N = 100$ sites.

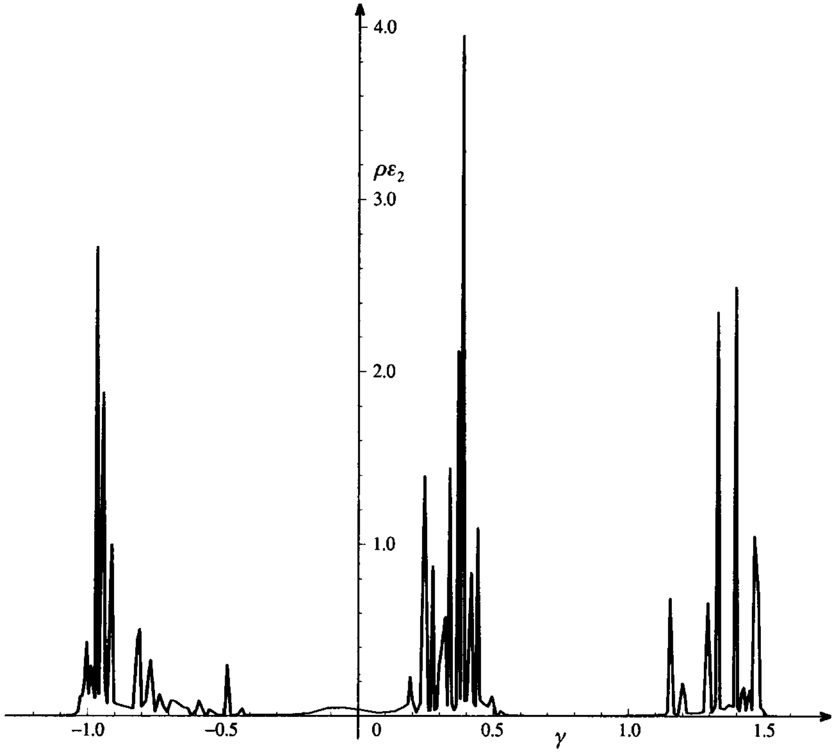

Fig. 2. Local density of states at site $s = 5$ plotted against γ for a one-dimensional next-nearest-neighbour tight-binding system of $N = 100$ sites with $\xi = 0.5$.

$$\langle s|\hat{G}(N;\gamma)|j\rangle = -\frac{b(s,j)}{\varepsilon_n}. \tag{39}$$

The local density of states $\rho(N,s;\gamma)$ at site s is given by

$$\rho(N,s;\gamma) = -\lim_{\delta\to 0+} \frac{\Im\{\langle s|\hat{G}(N,\gamma+\mathrm{i}\delta)|s\rangle\}}{\pi}. \tag{40}$$

For the nearest-neighbour model ($n = 1$) the diagonal elements of the Green's function are given, from (25), as

$$\langle s|\hat{G}(N;\gamma)|s\rangle = -\frac{\cos\{(N+1)\theta\} - \cos\{(N+1-2s)\theta\}}{2\varepsilon_1 \sin\theta \sin\{(N+1)\theta\}}, \tag{41}$$

where, from (23), $\theta = \arccos\gamma$. As an example, a plot of $\rho(100,5;\gamma)$ is shown in Fig. 1. In computing this curve δ was chosen to have the value 0.001. Since the density of states for real γ is, as indicated in (40), given by the limit $\delta \to 0$, the effect of a small non-zero δ is to replace delta function singularities by steep lorentzians.

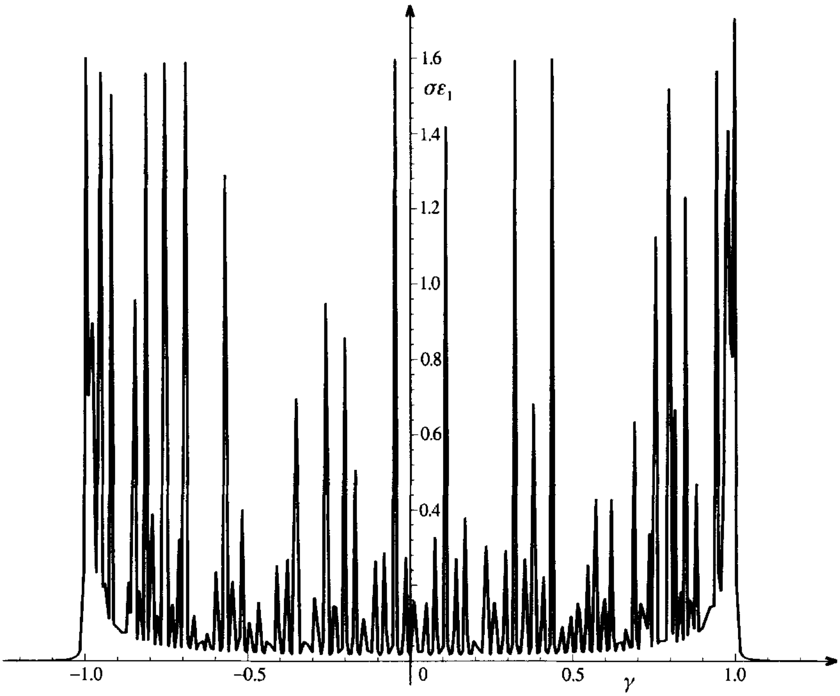

Fig. 3. Mean density of states plotted against γ for a one-dimensional nearest-neighbour tight-binding system of $N = 100$ sites.

A similar analysis applies to the next-nearest-neighbour chain ($n = 2$), using formulae (33), (35) and (36) for $b(s, j)$, where, from (27),

$$\cos\theta_{1,2} = -\tfrac{1}{4}\{\xi \pm \sqrt{\xi^2 + 8(1+\gamma)}\}, \tag{42}$$

with $\xi = \varepsilon_1/\varepsilon_2$. A plot of $\rho(100, 5; \gamma)$ for this model with $\xi = 0.5$ is shown in Fig. 2. Again δ has the value 0.001.

The local density of states at site s of a semi-infinite chain would be given in the limit of large N and the result for an infinite homogeneous chain is obtained by the second limit $s \to \infty$. Alternatively the limit as $N \to \infty$ of the mean density of states

$$\sigma(N;\gamma) = \frac{1}{N}\sum_{s=1}^{N}\rho(N, s; \gamma) \tag{43}$$

will yield the result for an infinite homogeneous chain. A plot of $\sigma(100; \gamma)$ for the nearest neighbour model is shown in Fig. 3. The well-known basin-shaped curve [6] for the density of states of the infinite homogeneous system is clearly seen with delta singularities, arising from the finite value of N, superimposed.

5. Conclusions

In this paper we have extended the work of Hu and O'Connell [5] by developing a method which will give an analytic formula for inverse of any finite $N \times N$ symmetric Toeplitz matrix of band-width $2n + 1 \leq 2N - 1$. The matrix size N enters the formula as a parameter and does not affect the complexity of the calculation. The only explicit matrix inversion that is required is of an $n \times n$ matrix. Since in most problems of interest n will be much smaller than N, the matrix inversion can be easily performed using an algebraic computing package.

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REFERENCES

[1] Calderón A., Spitzer F. and Widom H.: *Ill. J. Math.* **3** (1959), 490.
[2] Widom H.: *Ill. J. Math.* **4** (1960), 88.
[3] Golub G. H. and Van Loan C. F.: *Matrix Computations*, Johns Hopkins University Press, 1989.
[4] Streater R. F.: *Bull. London Math. Soc.* **11** (1979), 354.
[5] Hu G. Y. and O'Connell R. F.: *J. Phys. A: Math. Gen.* **29** (1996), 1511.
[6] Economou E. N.: *Green's Functions in Quantum Physics*, Springer Series in Solid-State Sciences 7, Springer, New York 1983.
[7] Southern B. W., Kumar A. A., Loly P. D. and Tremblay A-M. S.: *Phys. Rev. B* **27** (1983), 1405.
[8] Southern B. W., Kumar A. A. and Ashraff J. A.: *Phys. Rev. B* **28** (1983), 1785.
[9] Southern B. W., Liu T. S. and Lavis D. A.: *Phys. Rev. B* **39** (1989), 160.
[10] Cyr S. L. M., Southern B. W. and Lavis D. A.: *J. Phys.: Condens. Matter* **8** (1996), 4781.