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The maximum eigenvalue for a special matrix of order n

J Vila

Instituto de Matematica Aplicada San Luis, Universidad Nacional
de San Luis — CONICET, Chacabuco y Pedernera, 5700 San Luis, Argentina

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Abstract. The main objective of this paper is to find an analytic expression for the maximum eigenvalue of a special matrix A of order n , with n in the range $2 \leq n < \infty$. This will be done using a new result which states that if we know any entry $C_{ki}(j)$ of any real positive square matrix C^j (where j denotes the number of iterations), then we know, after taking the thermodynamic limit ($\lim j \rightarrow \infty$), the maximum eigenvalue of this matrix.

The analysis that we present in this paper is of particular interest, because the structure of the above-mentioned matrix A appears in several problems related to physical and biophysical systems in one dimension, i.e. the one-dimensional fluid model, denaturation of DNA (where we take loop entropy into account), in the study of the homogeneous island model, etc.

As a particular application of this method, we derive the Takahashi equation of state, which is the more general solution for a one-dimensional fluid model when we assume that the interaction potential between nearest-neighbour particles is arbitrary.

1. Introduction

As is well known, if we want to have intensive thermodynamic variables which are independent of the shape of the container, we must analyse physical (or biophysical) problems in the thermodynamic limit. Furthermore, it is known that in this limit only the maximum eigenvalue of the grand partition function (GPF) is of interest (when we can write this ensemble as a matrix product). However, as is also known, there are very difficult problems in computing the maximum eigenvalue when the order of the matrix is greater than 3×3 (in the case of 4×4 matrices, only in some special cases is it possible to find an analytic solution for the maximum eigenvalue). Bearing this in mind, in a previous paper [1] we found the maximum eigenvalue for a fourth-order matrix, which turned out to be of special interest in the analysis of potentiometric titration of polyelectrolytes [2]. As an extension of this method, in this paper we find the maximum eigenvalue of a special matrix A that appears when we study many physical and biophysical problems.

In § 2, we give the structure of the matrix A which appears when we analyse the denaturation of DNA [3] (if we take into account loop entropy) or as Poland and Scheraga also show, when we study a one-dimensional fluid model. Furthermore, in this section we show that the structure of the matrix also appears in the study of the island model [6]. Before proceeding to applications we will prove rigorously that in the thermodynamic limit, if we know any entry $C_{ki}(j)$ where j denotes the number of

iterations of C^j , then we know an analytic expression for the maximum eigenvalue of any real square matrix C . Finally, the remainder of § 2 (and § 3) are devoted to the application of this method for solving a problem of physical interest, i.e. the one-dimensional fluid model.

In § 3, we find the expression $a_{11}(j)$ of the A^j for the one-dimensional fluid model, in the special case that the interaction potential between nearest-neighbour particles is given by a square-well potential. In the same section we prove that the same expression for the maximum eigenvalue can be obtained using a classical method, which gives us confidence in our approach.

In § 4, we compute the maximum eigenvalue for the matrix A for any order n in the range $2 \leq n < \infty$, when we assume in the above-mentioned problem that the potential interaction between nearest-neighbour particles is arbitrary, and we obtain the Takahashi [5] equation of state as a special case.

We think that the analysis developed here might lead to a good workable method for studying more complex matrices. However, our primary interest here is to illustrate one alternative technique to find the maximum eigenvalue of one special matrix.

2. The structure of the matrix A

The structure of the matrix A , which represents many physical and biophysical problems (depending on the definition of the entries, as explained below) is given by

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1,n-2} & a_{1,n-1} & a_{1,n} \\ a_{21} & 0 & \dots & 0 & 0 & 0 \\ 0 & a_{32} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & a_{n-1,n-2} & 0 & 0 \\ 0 & 0 & \dots & 0 & a_{n,n-1} & a_{n,n} \end{pmatrix}. \quad (1)$$

In the matrix treatment for a finite chain in the homogeneous perfect-matching model [3], the above structure appears with the entries defined as $a_{11} = s$, $a_{1,k} = s\sigma_0\delta(k-1)$ for $k = 2, 3, \dots, n-1$, $a_{1,n} = s_{re}$, $a_{k+1,k} = 1$, for $k = 1, 2, \dots, n-1$ and $a_{n,n} = 1_{re}$ (where 're' indicates that the matrix element so designated will always contribute to the statistical weight of the right-hand free chain end of the molecule). The factor $\delta(i)$ gives the statistical weight for all possible loop sizes (the definition of the other factors, s , σ_0 , etc, can be found in [3]). It is important to mention that the fact that the double-stranded helix denatures by forming loops (in addition to a possible unwinding from the end) is, as Poland and Scheraga [3] say, one of the most important features of this model. Furthermore, the loop formation is also the most difficult feature of the model to treat.

On the other hand, the importance of taking medium-range as well as short-range interactions into account in the statistical mechanics treatment of the alpha helix and extended structures in proteins is well known [4]. It is possible to take into account the two types of interaction through an island model [6], as we see below, and in this case the structure of the matrix A given in equation (1) appears again. In the island model, the following assumption is made: the i th and $(i+l)$ th residues in the chain can interact with each other if and only if all of the i th to $(i+l)$ th residues are in the same state, ξ for example (where ξ could represent an alpha helix state). In this model,

we assume that there cannot be any interaction between a residue in a ξ state and a residue in another state χ (where χ could represent a coil state) or between two residues in the χ state. In this model, if we assign the statistical weights e_0 and 1 to the states ξ and χ , respectively, and the statistical weights e_p and 1 to interacting and non-interacting pairs of i th and $(i+l)$ th residues for $1 \leq p \leq l$, respectively, we find that the matrix that appears in this problem is given by the same matrix as in equation (1) with the entries defined in this case as $a_{1,k} = 1$ for $1 \leq k \leq n$, $a_{k+1,k} = E_k$ for $k = 1, 2, \dots, n-1$ and $a_{n,n} = E_n$ where $E_k = E_{k-1}e_k$ and $E_0 = e_0$.

Finally, we mention that, as Poland and Scheraga [3] show, it is possible to obtain the structure of the matrix A when we study a one-dimensional fluid model. In this model, the GPF can be written as a matrix product, where the matrix A is given by equation (1) for each site, with $a_{1k} = yq_k$ for $k = 1, 2, \dots, n$ and $a_{k+1,k} = 1$ for $k = 1, 2, \dots, n-1$ and $a_{n,n} = 1$. Here the fugacity y is given by: $y = \lambda\delta\Delta^{-1}$. Δ^{-1} appears from the momentum integral for each particle, $\lambda = \exp(-\beta\mu)$ appears from the construction of the GPF, and δ represents the lattice constant in this model (i.e. if L represents the length of the one-dimensional lattice, then the number of sites is $j = L\delta^{-1}$) and q_k is a Boltzmann factor assigned to a pair of particles separated by k sites, i.e. $q_k = \exp(-\beta\phi(kr_0\delta))$, where $(r_0\delta)$ represents the distance between lattice sites and $\phi(r)$ is an arbitrary potential, with $r = r_0k\delta$.

The model fluid treated by these authors has some intrinsic interest, firstly, because they approach the continuum by a variable lattice δ , thus allowing us to see the accuracy of the lattice model and, secondly, because in the thermodynamic limit (after taking the continuum limit $\delta \rightarrow 0$) it is possible to derive the Takahashi [5] equation of state. For these reasons, in the next section we compute the maximum eigenvalue of the matrix A , when the entries are defined as in the last problem, i.e. for the one-dimensional fluid. To do this we use the same method that we introduced earlier [1], i.e. through $a_{ki}(j)$, where j denotes the number of iterations of the A^j matrix. In the following we prove that the next statement is valid.

Let C be any real positive square matrix. Then there exist (k, l) such that

$$\lim_{j \rightarrow \infty} (1/j) \ln \Xi = \lim_{j \rightarrow \infty} (1/j) \ln C_{kl}(j) = \ln \lambda_{\max}$$

where λ_{\max} is the maximum eigenvalue of C which is necessarily real and positive.

From a statistical mechanics point of view, it is known that, in terms of the matrix C^j , the grand partition function (GPF) is given for the next expression:

$$\Xi = UC^jV \tag{2}$$

where U and V are appropriated vectors.

Taking into account the above relation, then (if we assume that C is diagonalisable) the next relation is valid too:

$$\Xi = U\Pi\Delta^j\Pi^{-1}V \quad \text{because} \quad C = \Pi\Delta\Pi^{-1} \tag{3a}$$

where Π and Π^{-1} are appropriated matrices that satisfy $\Pi\Pi^{-1} = I$ and Δ is given by

$$\Delta = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}$$

where λ will be an eigenvalue of C if and only if $\det|C - \lambda I| = 0$.

Then the GPF, as given by equation (2), can be rewritten as

$$\Xi = \sum_{p=1}^n \sum_{r=1}^n u_{1p}C_{pr}(j)v_{r1}. \tag{3b}$$

Taking the natural logarithm, we find

$$\frac{1}{j} \ln \Xi = \frac{1}{j} \ln C_{kl}(j) + \frac{1}{j} \ln \left(\sum_{p=1}^n \sum_{r=1}^n \frac{u_{1p} C_{pr}(j) v_{r1}}{C_{kl}(j)} \right).$$

In the last expression for the GPF we can rewrite $C_{kl}(j)$ using the relation given in equation (3a) as

$$C_{kl}(j) = \sum_{s=1}^n t_{k,l}^s \lambda_s^j \tag{3c}$$

where λ are the eigenvalues of the matrix C and t are coefficients. Arranging the eigenvalues in the following manner (and taking their absolute values, since some of them can be complex):

$$\lambda_1 \geq |\lambda_2| \geq |\lambda_3| \geq \dots \geq |\lambda_n|$$

it is easy to see that

$$\lim_{j \rightarrow \infty} (1/j) \ln \Xi = \lim_{j \rightarrow \infty} (1/j) \ln C_{kl}(j) = \ln \lambda_{\max} \tag{4}$$

because in the thermodynamic limit, $|\lambda_i/\lambda_{\max}|^j \rightarrow 0$ or 1 if $\lambda_{\max} > \lambda_i$ or $\lambda_{\max} = \lambda_i$ for the order of the matrix n , in the range $2 \leq n < \infty$.

We pause here to point out some important facts related to the proof of the last statement†. First, if we identify λ_{\max} with λ_1 , then t_{kl}^1 in equation (3c) cannot be zero for all (k, l) , otherwise C would be independent of its maximum eigenvalue. Secondly, we assume in the proof that C is diagonalisable, i.e. C possesses a complete set of eigenvectors and they become the columns of Π . However, in some special cases some eigenvectors are missing and a diagonal form is impossible. In such a case we want to choose some matrix M so that $M^{-1}CM$ will be as nearly diagonal as possible. The result of this effort of diagonalisation is the Jordan form: $J = M^{-1}CM = \Lambda$, with J entirely made up of blocks J_i , where each Jordan block is a triangular matrix with only one single eigenvalue [7]. Then we can use these properties to show that a similar proof for the statement works if C is not diagonalisable. Thirdly, we can state that the last statement is valid generically for all (k, l) and would only fail for a particular (k, l) in a pathological case.

Since our special matrix A of order n is non-negative for all the cases and, given the structure of A , it is not difficult to prove that for $j \geq n$, where n is the order of the square matrix A , A^j is a positive matrix. Next we prove the last statement. Consider the matrix A , with entries $a_{kk}(1)$ defined as $a_{kl}(1) > 0$ for $k = 1$ and $1 \leq l \leq n$, $a_{k+1,k}(1) > 0$ for $1 \leq k \leq n - 1$ and $a_{n,n}(1) > 0$.

Therefore, by the definition of the matrix product

$$a_{kl}(j) = \sum_{p=1}^n a_{kp} a_{pl}(j-1) \quad \forall j > 1$$

it is easy to see that for $j = 2$, the entries of A^2 satisfy

$$\begin{aligned} a_{kl}(2) &> 0 && \text{for } k = 1, 2; 1 \leq l \leq n \\ a_{k+2,k}(2) &> 0 && \text{for } 1 \leq k \leq n - 2 \\ a_{n,n}(2) &> 0 \end{aligned}$$

† I wish to express my gratitude to the referee for pointing this out.

and for $j = 3$, the entries of A^3 satisfy

$$\begin{aligned} a_{kl}(3) &> 0 && \text{for } k = 1, 2, 3; 1 \leq l \leq n \\ a_{k+3,k}(3) &> 0 && \text{for } 1 \leq k \leq n - 3 \\ a_{n,n} &> 0. \end{aligned}$$

From this, we find that the following relation is valid for $j \geq n$:

$$a_{kl}(j) > 0 \quad \text{for } 1 \leq k \leq n, 1 \leq l \leq n.$$

In such a case we can say that A^j for $j \geq n$ is a positive matrix.

In the one-dimensional fluid model, $a_{kl}(j)$ represents the (k, l) entry in the matrix A^j and, using the result obtained in a previous paper [1], we can write $a_{kl}(j)$ as

$$\begin{aligned} a_{kl}(j) &= a_{kk}a_{kl}(j-1) + a_k a^k a_{kl}(j-2) + \dots + a_k \bar{A}^{j-3} a^k a_{kl}(1) + a_k \bar{A}^{j-2} a^1 \\ &= \sum_{i=1}^{j-1} C_i^j a_{kl}(i) + \beta_{kl}(j-2) \quad \text{for } j > 1 \end{aligned} \tag{5}$$

with

$$\begin{aligned} C_{j-p}^j &= a_k \bar{A}^{p-2} a^k && p > 2 \\ C_{j-1}^j &= a_{kk} \end{aligned} \tag{6}$$

where the matrix \bar{A} is obtained from A by deleting the row k and the column k . The vector a_k is the k th row of A with the element k deleted. Similarly, a^m is the m th column of A without the entry k , for $m = k, l$. The products are matrix products and scalar products.

The recursion relation given in the above equation can be solved by making use of the general iterative method developed in [8], and the solution can be written as follows:

$$\begin{aligned} a_{kl}(j) &= \left(\sum_{r=1}^{j-1} \sum_{(l_1, \dots, l_r)' \in E_r^{j-1}} a_{(l_1, \dots, l_r)'}^j \right) a_{kl}(1) + \left[\sum_{i=2}^{j-1} \left(\sum_{r=1}^{j-i} \sum_{(l_1, \dots, l_r)' \in E_r^{j-i}} a_{(l_1, \dots, l_r)'}^j \right) \beta_{kl}(i) \right] \\ &\quad + \beta_{kl}(j-2) \quad \text{for } j > 1 \end{aligned} \tag{7}$$

$$\begin{aligned} E_r^{j-i} &= \left\{ (l_1, \dots, l_r): \sum_{i=1}^r l_i = j-1, l_i > 0 \text{ and integers} \right\} \\ a_{(l_1, \dots, l_r)'}^j &= C_{j-l_1}^j C_{j-l_1-l_2}^{j-l_1} \dots C_{j-j}^{j-l_1-l_2-\dots-l_{r-1}}. \end{aligned} \tag{8}$$

Given the structure of matrix A , we resolve equation (5) using equations (7) and (8) for the entry $a_{11}(j)$ of the A^j . The entry $a_{11}(j)$ is obtained using equation (7) as follows. The submatrix \bar{A} is given by

$$\bar{A} = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 1 \end{pmatrix} \tag{9}$$

where

$$a_1 = (\varepsilon_2 \varepsilon_3 \varepsilon_4 \dots \varepsilon_n) \quad a^1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{10}$$

In this application, we recall that the entries are defined as $\varepsilon_k = yq_k$ for $1 \leq k \leq n$, and if we take into account equation (6) and the structure of the vectors a_1 and a^1 , it is easy to see that only the $a_{j,1}(j-1)$ entry of \bar{A}^{j-1} for $1 < j \leq n-2$ is of interest. With these considerations it is easy to see that the submatrices \bar{A}^j for $1 < j \leq n-2$ are given by

$$\bar{A}^1 = \begin{pmatrix} 0 & \dots \\ 1 & \dots \\ 0 & \dots \\ \vdots & \dots \\ 0 & \dots \end{pmatrix} \quad \bar{A}^2 = \begin{pmatrix} 0 & \dots \\ 0 & \dots \\ 1 & \dots \\ \vdots & \dots \\ 0 & \dots \end{pmatrix} \dots \bar{A}^{n-2} = \begin{pmatrix} 0 & \dots \\ 0 & \dots \\ 0 & \dots \\ \vdots & \dots \\ 1 & \dots \end{pmatrix}. \tag{11}$$

It is important to note that $a_{n,1}(j) = 1$ for $j \geq n-2$.

The element C_{j-l}^j defined in equation (6) is then given by

$$\begin{aligned} C_{j-l}^{j-p} &= a_1 A^{l-p-2} a^1 = \varepsilon_{l-p} & l \geq p+2 \\ C_{j-l}^{j-p} &= a_{11} & l = p+1 \end{aligned} \tag{12}$$

for $0 \leq p \leq j-2$. Then, using equation (8) and taking $r=1$, we obtain

$$\begin{aligned} \sum_{i=1}^1 l_i &= j-1 & \text{for } l_i > 0 \\ a_{(l_1, \dots, l_r)}^j &= C_{j-l_1}^j = C_1^j = \varepsilon_{j-1}. \end{aligned} \tag{13}$$

Carrying on with this analysis, we obtain for $r=2$:

$$\sum_{i=1}^2 l_i = j-1 \quad l_i > 0. \tag{14}$$

The following cases can be noted for this value of r :

(i) $l_1 = 1$ and $l_2 = j-2$:

$$a_{(l_1, \dots, l_r)}^j = C_{j-l_1}^j C_{j-(l_1+l_2)}^{j-l_1} = C_{j-1}^j C_1^{j-1} = \varepsilon_1 \varepsilon_{j-2} \tag{15}$$

(ii) $l_1 = j-2$ and $l_2 = 1$:

$$a_{(l_1, \dots, l_r)}^j = C_{j-l_1}^j C_{j-(l_1+l_2)}^{j-l_1} = C_2^j C_1^2 = \varepsilon_{j-2} \varepsilon_1. \tag{16}$$

It should be observed that the same expression is obtained by permuting the l in equation (16). Then, all combinations of l_1 and l_2 can be written in the following form:

$$\sum_{l_1=1}^{j-2} \varepsilon_{l_1} \varepsilon_{j-l_1-1}. \tag{17}$$

Then we obtain, for $r=3$,

$$\sum_{i=1}^3 l_i = j-1 \quad \text{for } l_i > 0. \tag{18}$$

In this case, as in the previous case, we must consider all the permutations of l . For example, for l_1, l_2 and l_3 we obtain

$$l_1 = 1, l_2 = 1, l_3 = j-3: \quad a_{(l_1, \dots, l_r)}^j = C_{j-1}^j C_{j-2}^{j-1} C_1^{j-2} = \varepsilon_1 \varepsilon_1 \varepsilon_{j-3} \tag{19}$$

$$l_1 = j - 3, l_2 = 1, l_3 = 1: \quad a_{(l_1, \dots, l_r)}^{j-1} = C_3^j C_2^3 C_1^2 = \varepsilon_{j-3} \varepsilon_1 \varepsilon_1. \quad (20)$$

It is not difficult to see that in this case we obtain one expression equivalent to equation (18) and it is given by

$$\sum_{l_1=1}^{j-3} \sum_{l_2=1}^{j-l_1-2} \varepsilon_{l_1} \varepsilon_{l_2} \varepsilon_{j-(l_1+l_2)-1}. \quad (21)$$

Then, following with this procedure, it is clear that for the general case, $r = k$, the corresponding expression will be

$$\sum_{l_1=1}^{j-k} \sum_{l_2=1}^{j-l_1-(k-1)} \dots \sum_{l_{k-1}=1}^{j-(l_1+l_2+\dots+l_{k-2})-2} \varepsilon_{l_1} \varepsilon_{l_2} \dots \varepsilon_{j-(l_1+\dots+l_{k-1})-1}. \quad (22)$$

Using the above relations, we can find that the entry $a_{11}(j)$ is given by

$$\begin{aligned} a_{11}(j) = & \sum_{r=1}^{j-1} \left(\sum_{l_1=1}^{j-r} \sum_{l_2=1}^{j-l_1-r+1} \dots \sum_{l_{r-1}=1}^{j-(l_1+\dots+l_{r-2})-2} \varepsilon_{l_1} \varepsilon_{l_2} \dots \varepsilon_{j-(l_1+l_2+\dots+l_{r-1})-1} \right) \varepsilon_1 \\ & + \left[\sum_{i=2}^{j-1} \left(\sum_{r=1}^{j-i} \sum_{l_1=1}^{j-r-i} \dots \sum_{l_{r-1}=1}^{j-(l_1+\dots+l_{r-2})-2-i} \varepsilon_{l_1} \varepsilon_{l_2} \dots \varepsilon_{j-(l_1+\dots+l_{r-1})-i} \right) \varepsilon_i \right] \\ & + \varepsilon_{j-2}. \end{aligned} \quad (23)$$

Equation (23) represents an analytic expression for the entry $a_{11}(j)$ of the matrix \mathbf{A}^j for $j \geq 2$. Naturally, if we are interested in the thermodynamic limit, this expression represents the maximum eigenvalue of the matrix \mathbf{A} . In this limit, the following property results:

$$\mathbf{A}^j = \begin{pmatrix} 0 & \dots \\ 0 & \dots \\ \vdots & \dots \\ \vdots & \dots \\ 1 & \dots \end{pmatrix} \quad \text{for every } j \geq n - 2 \quad (24)$$

as we can see through equation (11). Then

$$\varepsilon_{l-p} = \varepsilon_n \quad \text{for every } l - p \geq n - 2 \quad (25)$$

where ε_n corresponds to the entry $a_{1,n}$ of the matrix \mathbf{A} .

In the next section we find different expressions for the entry $a_{11}(j)$ given in equation (23), depending on the shape of the interaction potential, the value of the lattice parameter δ and the value of j (the number of iterations).

3. The solution for a square-well type potential

In what follows, we assume that the reader is familiar with [3], and we omit the discussion of many aspects related to the lattice model. In the one-dimensional fluid model we consider, as in [3], that each particle of the lattice is assigned the constant interparticle potential $\phi(k)$ over the interparticle distance $r_0\delta(k - \frac{1}{2})$ to $r_0\delta(k + \frac{1}{2})$. In the case where $\delta \rightarrow 0$ (as we will see in § 4), $\phi(k)$ approaches the smooth function $\phi(r)$, as we can see in figure 1. It is important to say that in this section we take $\delta = 1$, which represents a very poor approximation to the continuum, i.e. for $\delta \rightarrow 0$. However

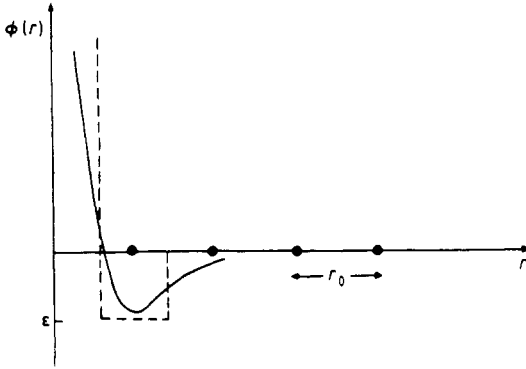


Figure 1. $\phi(r)$ for $\delta = 1$ (---) and $\delta \rightarrow 0$ (—).

our primary interest here is to illustrate the technique developed in § 2 and show that in the thermodynamic limit, $\lim_{j \rightarrow \infty} a_{11}(j)$ gives us the maximum eigenvalue of the GPF. Then we prove that this maximum eigenvalue can be obtained through a classical method, i.e. evaluating the secular equation given by $|\mathbf{A} - \lambda \mathbf{I}| = 0$.

In this simple application we assume that the interaction potential between nearest-neighbour particles is given by

$$\phi(r) = \begin{cases} \infty & r < r_0 \\ -\epsilon & r_0 \leq r < 2r_0 \\ 0 & r \geq 2r_0 \end{cases} \tag{26}$$

or, since $r = kr_0\delta$ for k lattice sites, $\phi(r) = 0$ and $q_k = 1$ for $k \geq n = 2/\delta$.

$n = 2$ defines, firstly, the order of the matrix \mathbf{A} , i.e. order two, and, secondly, the number of lattice sites beyond which the potential is truncated to zero, as we can see in figure 1.

With the above consideration in mind we next find an analytic expression for $a_{11}(j)$, valid for any $j \geq 2$, and then we will find the maximum eigenvalue taking the thermodynamic limit, i.e. using the relation, given by equation (4),

$$\lim_{j \rightarrow \infty} (1/j) \ln a_{kl}(j) = \ln \lambda_{\max}.$$

It is useful to remember that every entry of the matrix \mathbf{A}^j can be written as

$$a_{kl}(j) = \sum_{i=1}^{j-1} C_i^j a_{kk}(i) + \beta_{kl}(j-2) \tag{27}$$

$$a_{kl}(j-1) = \sum_{i=1}^{j-2} C_i^{j-1} a_{kl}(i) + \beta_{kl}(j-3).$$

If $\delta = 1$, then

$$a_1 = \epsilon_2 \quad a^1 = 1 \quad \bar{\mathbf{A}} = 1 \tag{28}$$

and the coefficients will be given by

$$C_{j-l}^{j-p} = a_{\perp} \bar{\mathbf{A}}^{l-p-2} a^{\perp} = \epsilon_2 \quad l \geq p+2 \tag{29}$$

$$C_{j-l}^{j-p} = \epsilon_1 \quad l = p+1$$

$$\beta_{kl}(j-p) = a_k \bar{\mathbf{A}}^{j-p} a^l = \epsilon_2 \quad \forall 0 \leq p \leq j. \tag{30}$$

Writing $a_{kl}(j)$ and $a_{kl}(j-1)$ explicitly

$$a_{kl}(j) = C_{j-1}^j a_{kl}(j-1) + C_{j-2}^j a_{kl}(j-2) + \sum_{i=1}^{j-3} C_i^j a_{kl}(i) + \beta_{kl}(j-2) \tag{31}$$

$$a_{kl}(j-1) = C_{j-2}^{j-1} a_{kl}(j-2) + \sum_{i=1}^{j-3} C_i^{j-1} a_{kl}(i)$$

it can be seen from equation (29) that

$$\sum_{i=1}^{j-3} C_i^j a_{kl}(i) = \sum_{i=1}^{j-3} C_i^{j-1} a_{kl}(i) \tag{32}$$

and using this result it is easy to write $a_{kl}(j)$ as

$$a_{kl}(j) = (1 + C_{j-1}^j) a_{kl}(j-1) + (C_{j-2}^j - C_{j-2}^{j-1}) a_{kl}(j-2) + \beta_{kl}(j-2) - \beta_{kl}(j-3). \tag{33}$$

From equation (30) it is clear that

$$\beta_{kl}(j-2) = \beta_{kl}(j-3) \quad \text{for } j \geq 2$$

and then

$$a_{kl}(j) = \bar{C}_{j-1}^j a_{kl}(j-1) + \bar{C}_{j-2}^j a_{kl}(j-2)$$

$$a_{kl}(1) = C_0^1 a_{kl}(0) \tag{34}$$

$$a_{kl}(0) = \varepsilon_1$$

where the coefficients are given by

$$\bar{C}_{j-l}^{j-p} = \begin{cases} 0 & l-p \geq 3 \\ \alpha & l-p = 1 \\ \gamma & l-p = 2 \end{cases} \quad \text{with } C_0^1 = \pi \tag{35}$$

where

$$\alpha = (1 + \varepsilon_1) \quad \gamma = (\varepsilon_2 - \varepsilon_1) \quad \pi = (\varepsilon_1^2 + \varepsilon_2) / \varepsilon_1. \tag{36}$$

Applying equation (7) to solve the recurrence given by equation (34), it is not difficult to see that $a_{(l_1, \dots, l_r)^j}$ is zero for $r < j/2$.

For $r \geq j/2$ the following cases are noted:

(i) if $r = j/2$: $\sum_{r=1}^{j/2} l_r = j$, $l_r > 0$ and integer:

$$a_{(l_1, \dots, l_r)^j} = C_{j-2}^j C_{j-4}^{j-2} \dots C_0^2 = \gamma^{j/2} \tag{37}$$

(ii) if $r = j/2 + 1$: $\sum_{r=1}^{j/2+1} l_r = j$, $l_r > 0$ and integer:

$$a_{(l_1, \dots, l_r)^j} = \begin{cases} C_{j-2}^j C_{j-4}^{j-2} \dots C_1^2 C_0^1 = \gamma^{j/2-1} \alpha \pi \left(\frac{(j/2+1)!}{(j/2-1)!1!1!} \right) \\ C_{j-2}^j C_{j-4}^{j-2} \dots C_2^3 C_0^2 = \gamma^{j/2-1} \alpha^2 \left(\frac{(j/2+1)!}{(j/2-1)!2!} \right). \end{cases} \tag{38}$$

The terms in brackets represent all permutations of l , which give the same result.

For the general case $r = j/2 + p$ the following expression is easily deduced:

$$a_{\{1, \dots, l\}'}^j = \begin{cases} C_{j-2}^j \dots C_0^1 = \gamma^{j/2-p} \alpha^{2p-1} \pi \left(\frac{(j/2+p)!}{(j/2-p)!(2p-1)!1!} \right) & (39) \\ C_{j-2}^j \dots C_0^2 = \gamma^{j/2-p} \alpha^{2p} \left(\frac{(j/2+p)!}{(j/2-p)!(2p)!} \right). & (40) \end{cases}$$

Then using equation (7), we obtain for $a_{11}(j+1)$ the following expression:

$$a_{11}(j+1) = \left[\gamma^{j/2} + \alpha^{j-1} \pi + \sum_{p=1}^{j/2-1} \sum_{r=0}^1 \left(\frac{(j/2+p)!}{(j/2-p)!(2p-r)!r!} \right) \gamma^{j/2-p} \alpha^{2p-r} \pi \right]. \quad (41)$$

In the above expression the first term results from putting $r = j/2$ and the second from $r = j$.

Equation (41) is an analytic expression for $a_{11}(j+1)$ and is valid for every $j \geq 2$ even; a similar expression can be obtained for j odd.

If we are interested in computing the maximum eigenvalue through the relation given in equation (4), then we have to write equation (41) as

$$\frac{1}{j} \ln a_{11}(j) = \ln \alpha + \frac{1}{j} \ln \left(\frac{\gamma^{j/2}}{\alpha^j} + \frac{\pi}{\alpha} + \sum_{p=1}^{j/2-1} \sum_{r=0}^1 \frac{(j/2+p)!}{(j/2-p)!(2p-r)!r!} \gamma^{j/2-p} \alpha^{2p-r-j} \pi \right). \quad (42)$$

Taking into account that $\gamma/\alpha < 1$, equation (41) takes the form

$$\lim_{j \rightarrow \infty} \frac{1}{j} \ln a_{11}(j) = \ln \alpha + \frac{1}{j} \ln \left(\frac{(j/2+\bar{p})!}{(j/2-\bar{p})!(2\bar{p})!} \gamma^{j/2-\bar{p}} \alpha^{2\bar{p}-j} \right) \quad (43)$$

where \bar{p} is the value of p that maximises the sum given in equation (43),

$$\bar{p} = (j/2)\xi \quad \xi = (1 + 4\gamma/\alpha^2)^{-1/2}. \quad (44)$$

Replacing \bar{p} in equation (43) and using the Stirling approximation for $()!$ we obtain

$$\begin{aligned} \lim_{j \rightarrow \infty} (1/j) \ln a_{11}(j) &= \ln \alpha + (1/j)[(j/2)(1+\xi) \ln(j/2)(1+\xi) - (j/2)(1-\xi) \ln(j/2)(1-\xi) \\ &\quad - j\xi \ln j\xi + (j/2)(1-\xi) \ln \gamma + (j/2)(\xi-1) \ln \alpha^2] \end{aligned} \quad (45)$$

and using the equalities

$$\ln(1 \pm \xi) = \ln \xi + \ln(\xi^{-1} \pm 1) \quad (46)$$

equation (45) takes the form

$$\lim_{j \rightarrow \infty} (1/j) \ln a_{11}(j) = \ln \alpha + \ln(1 + \xi^{-1}) - \ln 2. \quad (47)$$

As can be easily demonstrated, the maximum eigenvalue λ_{\max} of the matrix A with $\delta = 1$ is given by equation (47), i.e. if we resolve the secular equation $|A - \lambda I| = 0$.

4. The solution for an arbitrary potential

In this section we find an analytic expression for the maximum eigenvalue of the matrix A of order $n = 2/\delta$, for any value of lattice parameter δ in the thermodynamic limit. As a particular case, we derive the Takahashi equation of state, i.e. when we let $\delta \rightarrow 0$. In this section we assume that the interaction potential is arbitrary among nearest-neighbour particles and the following relations are valid:

$$\phi(r) = \begin{cases} \infty & \text{for } r < r_0 \\ \phi(r) & \text{for } r_0 \leq r < 2r_0 \\ 0 & \text{for } r \geq 2r_0 \end{cases} \quad (48)$$

or, since $r = kr_0\delta$, $\phi(r) = 0$ for $k \geq n = 2/\delta$.

The following definitions, given by Poland and Scheraga [3], will be useful for the solution of this model. The number of sites j is equal to L/δ , where L is the length of lattice and δ is the lattice variable. Simultaneously the parameter j satisfies

$$\sum_{\sigma=1}^N k_{\sigma} = j \quad (49)$$

where N represents the number of particles in the system and σ is an index designating the number of the sequence of two particles in the lattice separated by k sites.

In terms of the above parameters the entries of the matrix A are given by

$$\epsilon_k = yq_k \quad \forall 1 \leq k \leq n \quad \text{with } q_n = 1. \quad (50)$$

n represents the number of lattice sites, beyond which the potential is truncated to zero, and it is not difficult to see that the matrix required for a given value of δ is $n \times n$.

Using the above definition we can see that the following relations are valid in the thermodynamic limit, i.e. for $j \rightarrow \infty$:

$$\lim_{j \rightarrow \infty} \sum_{r=1}^{j-1} (\sum \dots \sum) \epsilon_1 = \lim_{j \rightarrow \infty} \sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}} \quad (51)$$

for the first term of $a_{11}(j)$ given in equation (23). It is not difficult to see that in the above expression each combination of the first term appears as a particular case of the second term when we let $j \rightarrow \infty$. Also, the following inequality is valid†:

$$\lim_{j \rightarrow \infty} \sum_{i=2}^{j-1} \left(\sum_{r=1}^{j-i} \sum \dots \sum \right) \epsilon_i < \lim_{j \rightarrow \infty} \left[j \sum_{N=1}^j \left(\prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}} \right) yq_i \right] \quad (52)$$

because the term $(yq_{k_{\sigma}})$ satisfies $yq_{k_{\sigma}} > 0 \forall k_{\sigma}$.

Then we can say that for $j \rightarrow \infty$ the following is valid:

$$\lim_{j \rightarrow \infty} \frac{1}{j} \ln a_{11}(j) = \frac{1}{j} \ln \left(\sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}} \right) \quad (53)$$

since

$$\frac{1}{j} \ln \left(\frac{1 + j[\sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j (yq_{k_{\sigma}})(yq_i)]}{\sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}}} \right) \rightarrow 0 \quad (54)$$

† The inequality is valid for any value of the subscript i in the range $1 < i < j$.

when we take $\lim_{j \rightarrow \infty}$. Using equation (4), we can write the following relation for $a_{11}(j)$:

$$\lim_{j \rightarrow \infty} \frac{1}{j} \ln a_{11}(j) = \frac{1}{j} \ln \left(\sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}} \right) = \ln \lambda_{\max} \tag{55}$$

where, as is well known, the maximum eigenvalue is given by [3]

$$\lambda = \exp(\beta p \delta) \quad \text{as} \quad \lim_{j \rightarrow \infty} \Xi = e^{\beta p L} \rightarrow \lambda_{\max}^j. \tag{56}$$

In the above expression for λ_{\max} , p is the real pressure in the system and L is the volume, and we put λ^j as

$$\lambda^j = \exp(\beta p \delta j) = x^j.$$

Here

$$x^j = x^{\sum_{\sigma=1}^N k_{\sigma}} = \prod_{\sigma=1}^N x^{k_{\sigma}}. \tag{57}$$

Using equation (57) in equation (55) we obtain

$$\lim_{j \rightarrow \infty} \frac{1}{j} \ln \left(\sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}} \lambda^{-j} \right) = \frac{1}{j} \ln \left(\sum_{N=1}^j \prod_{\sigma=1}^N \sum_{k_{\sigma}=1}^j yq_{k_{\sigma}} x^{-k_{\sigma}} \right). \tag{58}$$

Since $yq_k x^{-k}$ depends only on the number of unoccupied sites between two particles and is independent of its location in the lattice, we can write equation (58) as

$$\lim_{j \rightarrow \infty} \frac{1}{j} \ln \left[\sum_{N=1}^j \left(\sum_{k=1}^j yq_k x^{-k} \right)^N \right] = 0. \tag{59}$$

From the point of view of physics, we can see the term $yq_k x^{-k}$ as the probability of finding two particles having k unoccupied lattice sites between them. Then we can say, without losing generality, that the following is valid:

$$\sum_{k=1}^{\infty} \frac{yq_k}{x^k} = 1. \tag{60}$$

On the other hand, from a mathematical point of view, the above relation also satisfies the condition given in equation (59).

Then, taking into account that the density ρ is given by the relation:

$$\rho = \frac{y}{x\delta} \left(\frac{\partial y}{\partial x} \right)^{-1} \tag{61}$$

we obtain, using equation (60), the following expression for ρ :

$$\rho = \frac{\sum_{k=1}^{\infty} q_k x^{-k}}{\sum_{k=1}^{\infty} (k\delta) q_k x^{-k}}. \tag{62}$$

Finally, if we let $\delta \rightarrow 0$, it is not difficult to prove that the equation of state is given by

$$\lim_{\delta \rightarrow 0} \rho = \frac{\int_0^{\infty} \exp[-\beta(pu + \phi(u))] du}{\int_0^{\infty} u \exp[-\beta(pu + \phi(u))] du}. \tag{63}$$

The above expression is the known Takahashi [5] equation of state for a one-dimensional fluid model, when we suppose that the interaction occurs only among nearest neighbours. Furthermore, from the above relation it is clear (as Takahashi also points out) that ρ must be a single-valued function of p . This means that the coexistence of two phases is impossible in a one-dimensional system for any choice of the potential (the same can be concluded from the theorem of Van Hove [9]).

5. Discussion

If we review the books devoted to matrix theory, we find that the eigenvalue problem is one of the outstanding successes of numerical analysis [7]. Nevertheless, until now no one has known how to solve it in analytic form for any case, because everything depends on the size and properties of the matrix and on the number of eigenvalues that are required. In particular, if we are interested in obtaining an analytic expression for the maximum eigenvalue (as in almost every physical and biophysical problem) we are of the opinion that the method used in this paper is useful.

On the other hand, if we are interested in bounded values of the eigenvalues of any matrix we can use the Gershgorin theorem† (the circle theorem [7]). However, this method does not give us an analytical expression for the maximum eigenvalue (only in certain cases is it possible to find a bound value of this). Finally, we think that both the method used in this paper and the Gershgorin theorem are useful, but with different final results.

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† The author wishes to thank the referee for pointing out this property.