Norm Estimates for Inverses of Toeplitz Distance Matrices

B. J. C. BAXTER

Department of Applied Mathematics and Theoretical Physics, Silver Street, Cambridge CB3 9EW, England

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A radial basis function approximation has the form

$$s(x)\sum_{j=1}^{n}y_{j}\varphi(\|x-x_{j}\|_{2}), \quad x \in \mathcal{R}^{d},$$

where $\varphi \colon [0,\infty) \to \mathcal{R}$ is some given function, $(y_j)_1^n$ are real coefficients, and the centres $(x_j)_1^n$ are points in \mathcal{R}^d . For a wide class of functions φ , it is known that the interpolation matrix $A = (\varphi(\|x_j - x_k\|_2))_{j,k=1}^n$ is invertible. Further, several recent papers have provided upper bounds on $\|A^{-1}\|_2$, where the points $(x_j)_1^n$ satisfy the condition $\|x_j - x_k\|_2 \ge \delta$, $j \ne k$, for some positive constant δ . In this paper, we provide the least upper bound on $\|A^{-1}\|_2$ when the points $(x_j)_1^n$ form any subset of the integer lattice \mathcal{Z}^d , and when φ is a conditionally negative definite function of order 1, a large set of functions which includes the multiquadric. Specifically, for any set of points $(x_j)_1^n \subset \mathcal{Z}^d$, we provide the inequality

$$||A^{-1}||_2 \le \left(\sum_{k \in \mathcal{F}^d} |\hat{\varphi}(||\pi e + 2\pi k||_2)|\right)^{-1},$$

where $e = [1, ..., 1]^T \in \mathcal{R}^d$ and where $\hat{\varphi}$ is the generalized Fourier transform of φ . We provide a constructive proof that no smaller bound is valid and comment on the relevance of the method of analysis to the problem of estimating *all* the eigenvalues of such an interpolation matrix. © 1994 Academic Press, Inc.

1. Introduction

The multivariate interpolation problem is as follows: given points $(x_j)_{j=1}^n$ in \mathscr{R}^d and real numbers $(f_j)_{j=1}^n$, construct a function $s:\mathscr{R}^d\to\mathscr{R}$ such that $s(x_k)=f_k$, for $k=1,\ldots,n$. The radial basis function approach is to choose a univariate function $\varphi\colon [0,\infty)\to\mathscr{R}$, a norm $\|\cdot\|$ on \mathscr{R}^d , and to let

s take the form

$$s(x) = \sum_{j=1}^{n} y_{j} \varphi(\|x - x_{j}\|). \tag{1.1}$$

The norm $\|\cdot\|$ will be the Euclidean norm throughout this paper. We see that the radial basis function interpolation problem has a unique solution for any given scalars $(f_j)_{j=1}^n$ if and only if the matrix $(\varphi(\|x_j-x_k\|))_{j,k=1}^n$ is invertible. Such a matrix will be called a distance matrix in this paper. These functions provide a useful and flexible form for multivariate approximation, but their approximation power as a space of functions is not addressed in this paper.

A powerful and elegant theory was developed by Schoenberg and others some 50 years ago which may be used to analyse the singularity of distance matrices. Indeed, in Schoenberg [9] it was shown that a Euclidean distance matrix, which arises when $\varphi(r) = r$, is invertible if $n \ge 2$ and the points $(x_i)_{i=1}^n$ are distinct. Further, extensions of this work by Micchelli [6] proved that the distance matrix is invertible for several classes of functions, including the Hardy multiquadric, the only restrictions on the points $(x_i)_{i=1}^n$ being that they are distinct and that $n \ge 2$. Thus the singularity of the distance matrix has been successfully investigated for many useful radial basis functions. In this paper, we bound the eigenvalue of smallest modulus for certain distance matrices. Specifically, we provide the greatest lower bound on the moduli of the eigenvalues in the case when the points $(x_i)_{i=1}^n$ form a subset of the integers \mathcal{Z}^d , our method of analysis applying to a wide class of functions which includes the multiquadric. More precisely, let N be any finite subset of the integers \mathcal{Z}^d and let λ_{\min}^N be the smallest eigenvalue in modulus of the distance matrix $(\varphi(||j-k||))_{i,k\in\mathbb{N}}$. Then the results of Sections 3 and 4 provide the inequality

$$|\lambda_{\min}^N| \geq C_{\varphi},$$

where C_{φ} is a positive constant for which an elegant formula is derived. We also provide a constructive proof that C_{φ} cannot be replaced by any larger number, and it is for this reason that we shall describe inequality (1.2) as an *optimal* lower bound. Similarly, we shall say that an upper bound is optimal if none of the constants appearing in the inequality can be replaced by smaller numbers.

It is crucial to our analysis that the distance matrix $(\varphi(||j-k||))_{j,k \in N}$ may be embedded in the bi-infinite matrix $(\varphi(||j-k||))_{j,k \in \mathcal{Z}^d}$. Such a bi-infinite matrix is called a Toeplitz matrix if d=1. We shall use this name for all values of d, since we use the multivariate form of the Fourier analysis of Toeplitz forms (see Grenander and Szegő [5]).

Of course, inequality (1.2) also provides an upper bound on the norm of the inverse of the distance matrices generated by finite subsets of the integers \mathcal{Z}^d . This is not the first paper to address the problem of bounding the norms of inverses of distance matrices and we acknowledge the papers of Ball [2] and Narcowich and Ward [7, 8], which first interested the author in such estimates. Their results are not limited to the case when the data points are a subset of the integers. Instead, they apply when the points satisfy the condition $||x_j - x_k|| \ge \varepsilon$ for $j \ne k$, where ε is a positive constant, and they provide lower bounds on the smallest modulus of an eigenvalue for several functions φ , including the multiquadric. We will find that these bounds are not optimal, except in the special case of the Euclidean norm in the univariate case. Further, our bounds apply to all the conditionally negative definite functions of order 1. The definition of this class of functions may be found in Section 3.

We shall often use the theory of generalized Fourier transforms in this paper, for which our principal reference will be the excellent book of Jones [4]. These transforms are precisely the Fourier transforms of tempered distributions constructed in Schwartz [10]. First, however, Section 2 presents several theorems which require only the classical theory of the Fourier transform. These results will be necessary in Section 3.

2. Toeplitz Forms and Theta Functions

We require several properties of the Fejér kernel, which is defined as follows. For each positive integer n, the nth univariate Fejér kernel is the positive trigonometric polynomial

$$K_n(t) = \sum_{k=-n}^{n} (1 - |k|/n) \exp(ikt)$$
$$= \frac{\sin^2 nt/2}{n \sin^2 t/2}.$$

Further, the nth multivariate Fejér kernel is defined by the product

$$K_n(t_1,\ldots,t_d) = K_n(t_1)K_n(t_2)\cdots K_n(t_d), \quad t = (t_1,\ldots,t_d) \in \mathcal{R}^d.$$
 (2.2)

Lemma 2.1. The univariate kernel enjoys the following property: for any continuous 2π -periodic function $f: \mathcal{R} \to \mathcal{R}$ and for all $x \in \mathcal{R}$ we have

$$\lim_{n \to \infty} (2\pi)^{-1} \int_0^{2\pi} K_n(t-x) f(t) dt = f(x).$$

Moreover, this kernel satisfies the equations

$$(2\pi)^{-1} \int_0^{2\pi} K_n(t) dt = 1$$
 (2.3)

and

$$K_n(t) = \left| n^{-1/2} \sum_{k=0}^{n-1} \exp(ikt) \right|^2.$$
 (2.4)

Proof. Most textbooks on harmonic analysis contain the first property and (2.3). For example, see p. 89ff of Vol. I of Zygmund [13]. It is elementary to deduce (2.4) from (2.1). ■

Lemma 2.2. For every continuous $[0, 2\pi]^d$ -periodic function $f: \mathcal{R}^d \to \mathcal{R}$, the multivariate Fejér kernel gives the convergence property

$$\lim_{n \to \infty} (2\pi)^{-d} \int_{[0,2\pi]^d} K_n(t-x) f(t) dt = f(x)$$

for every $x \in \mathcal{R}^d$. Further, K_n is the square of the modulus of a trigonometric polynomial with real coefficients and

$$(2\pi)^{-d} \int_{[0,2\pi)^d} K_n(t) dt = 1.$$

Proof. The first property is Theorem 1.20 of Chap. 17 of Zygmund [13]. The last part of the lemma is an immediate consequence of (2.3), (2.4) and the definition of the multivariate Fejér kernel.

All sequences will be real sequences in this paper. Further, we shall say that a sequence $(a_j)_{\mathcal{Z}^d} := \{a_j\}_{j \in \mathcal{Z}^d}$ is *finitely supported* if it contains only finitely many nonzero terms. The scalar product of two vectors x and y in \Re^d will be denoted by xy.

PROPOSITION 2.3. Let $f: \mathcal{R}^d \to \mathcal{R}$ be an absolutely integrable continuous function whose Fourier transform \hat{f} is also absolutely integrable. Then for any finitely supported sequence $(a_j)_{\mathcal{Z}^d}$, and for any choice of points $(x_j)_{\mathcal{Z}^d}$ in \mathcal{R}^d , we have the identity

$$\sum_{j,k\in\mathcal{Z}^d} a_j a_k f(x_j - x_k) = (2\pi)^{-d} \int_{\mathcal{R}^d} \left| \sum_{j\in\mathcal{Z}^d} a_j \exp(ix_j \xi) \right|^2 \hat{f}(\xi) d\xi.$$

Proof. The function $\mathscr{R}^d \ni x \mapsto \sum_{j,k} a_j a_k f(x + x_j - x_k)$ is absolutely integrable. Its Fourier transform is given by

$$\begin{split} \left[\sum_{j,\,k\in\mathcal{Z}^d} a_j a_k f(\cdot + x_j - x_k)\right] \hat{}(\xi) &= \sum_{j,\,k\in\mathcal{Z}^d} a_j a_k \exp(i(x_j - x_k)\xi) \hat{f}(\xi) \\ &= \left|\sum_{j\in\mathcal{Z}^d} a_j \exp(ix_j\xi)\right|^2 \hat{f}(\xi), \quad \xi \in \mathcal{R}^d, \end{split}$$

and is therefore absolutely integrable. Applying the Fourier inversion theorem, we have

$$\sum_{j,k\in\mathcal{Z}^d} a_j a_k f(x+x_j-x_k)$$

$$= (2\pi)^{-d} \int_{\mathcal{R}^d} \left| \sum_{j\in\mathcal{Z}^d} a_j \exp(ix_j \xi) \right|^2 \hat{f}(\xi) \exp(ix\xi) d\xi.$$

Setting x = 0 produces the stated equation.

In this paper, a key rôle will be played by the symbol function

$$\sigma(\xi) = \sum_{k \in \mathcal{Z}^d} \hat{f}(\xi + 2\pi k), \quad \xi \in \mathcal{R}^d.$$
 (2.5)

If $\hat{f} \in L^1(\mathcal{R}^d)$, then σ is an absolutely integrable function on $[0, 2\pi]^d$ and its defining series is absolutely convergent almost everywhere. These facts are consequences of the relations

$$\infty > \int_{\mathcal{R}^d} \left| \hat{f}(\xi) \right| d\xi = \sum_{k \in \mathcal{Z}^d} \int_{[0, 2\pi)^d} \left| \hat{f}(\xi + 2\pi k) \right| d\xi$$
$$= \int_{[0, 2\pi)^d} \sum_{k \in \mathcal{Z}^d} \left| \hat{f}(\xi + 2\pi k) \right| d\xi,$$

the exchange of integration and summation being a consequence of Fubini's theorem. If the points $(x_j)_{\mathcal{Z}^d}$ are integers, then we readily deduce the following bounds on the quadratic form $\sum_{j,k\in\mathcal{Z}^d}a_ja_kf(j-k)$.

PROPOSITION 2.4. Let f satisfy the conditions of Proposition 2.3 and let $(a_i)_{x^d}$ be a finitely supported sequence. Then we have the identity

$$\sum_{j,k\in\mathcal{Z}^d} a_j a_k f(j-k) = (2\pi)^{-d} \int_{[0,2\pi]^d} \left| \sum_{j\in\mathcal{Z}^d} a_j \exp(ij\xi) \right|^2 \sigma(\xi) d\xi.$$
 (2.6)

Further, letting $m = \inf\{\sigma(\xi): \xi \in [0, 2\pi]^d\}$ and $M = \sup\{\sigma(\xi): \xi \in [0, 2\pi]^d\}$, we have the bounds

$$m\sum_{j\in\mathcal{Z}^d}a_j^2\leq\sum_{j,\,k\in\mathcal{Z}^d}a_ja_kf(j-k)\leq M\sum_{j\in\mathcal{Z}^d}a_j^2.$$

Proof. Proposition 2.3 implies the equation

$$\sum_{j,k\in\mathcal{Z}^d} a_j a_k f(j-k)$$

$$= \sum_{k\in\mathcal{Z}^d} (2\pi)^{-d} \int_{[0,2\pi)^d} \left| \sum_{j\in\mathcal{Z}^d} a_j \exp(ij\xi) \right|^2 \hat{f}(\xi+2\pi k) d\xi$$

$$= (2\pi)^{-d} \int_{[0,2\pi)^d} \left| \sum_{j\in\mathcal{Z}^d} a_j \exp(ij\xi) \right|^2 \sigma(\xi) d\xi,$$

the exchange of integration and summation being justified by Fubini's theorem. For the upper bound, the Parseval theorem yields the expressions

$$\sum_{j,k\in\mathcal{Z}^d} a_j a_k f(j-k) = (2\pi)^{-d} \int_{[0,2\pi]^d} \left| \sum_{j\in\mathcal{Z}^d} a_j \exp(ij\xi) \right|^2 \sigma(\xi) d\xi$$

$$\leq M \sum_{j\in\mathcal{Z}^d} a_j^2.$$

The lower bound follows similarly and the proof is complete.

The inequalities of the last proposition enjoy the following optimality property.

PROPOSITION 2.5. Let f satisfy the conditions of Proposition 2.3 and suppose that the symbol function is continuous. Then the inequalities of Proposition 2.4 are optimal lower and upper bounds.

Proof. Let $\xi_M \in [0, 2\pi]^d$ be a point such that $\sigma(\xi_M) = M$, which exists by continuity of the symbol function. We shall construct a set $\{(a_j^{(n)})_{j \in \mathcal{Z}^d}: n = 1, 2, \ldots\}$ of finitely supported sequences such that $\sum_{j \in \mathcal{Z}^d} |a_j^{(n)}|^2 = 1$, for all n, and

$$\lim_{n \to \infty} \sum_{j,k \in \mathcal{Z}^d} a_j^{(n)} a_k^{(n)*} f(j-k) = M. \tag{2.7}$$

We recall from Lemma 2.2 that the multivariate Fejér kernel is the square of the modulus of a trigonometric polynomial with real coefficients. Therefore there exists a finitely supported sequence $(a_j^{(n)})_{\mathcal{L}^d}$ satisfying the relation

$$\left|\sum_{j\in\mathcal{Z}^d} a_j^{(n)} \exp(ij\xi)\right|^2 = K_n(\xi - \xi_M), \quad \xi \in \mathcal{R}^d. \tag{2.8}$$

Further, the Parseval theorem and Lemma 2.2 provide the equations

$$\sum_{j \in \mathcal{Z}^d} |a_j^{(n)}|^2 = (2\pi)^{-d} \int_{[0,2\pi]^d} K_n(\xi - \xi_M) d\xi = 1$$

and

$$\lim_{n\to\infty} (2\pi)^{-d} \int_{[0,2\pi]^d} K_n(\xi-\xi_M) \sigma(\xi) d\xi = \sigma(\xi_M) = M.$$

Now it follows from (2.6) and (2.8) that the limit (2.7) holds. The lower bound of Proposition 2.4 is dealt with in the same fashion.

The set of functions satisfying the conditions of Proposition 2.5 is nonvoid. For example, suppose that we have $\hat{f}(\xi) = \mathscr{O}(\|\xi\|^{-d-\delta})$, for large $\|\xi\|$, where δ is a positive constant. Then the series defining the symbol function σ converges uniformly, by the Weierstrass M-test, and σ is continuous, being a uniformly convergent sum of continuous functions. These remarks apply when f is a Gaussian, which is the subject of the rest of this section. We shall see that the analysis of the Gaussian provides the key to all the results of this paper.

PROPOSITION 2.6. Let λ be a positive constant and let $f(x) = \exp(-\lambda ||x||^2)$, for $x \in \mathcal{R}^d$. Then f satisfies the conditions of Proposition 2.5.

Proof. The Fourier transform of f is the function $\hat{f}(\xi) = (\pi/\lambda)^{d/2} \exp(-\|\xi\|^2/4\lambda)$, which is a standard calculation of the classical theory of the Fourier transform. It is clear that f satisfies the conditions of Proposition 2.3, and that the symbol function is the expression

$$\sigma(\xi) = (\pi/\lambda)^{d/2} \sum_{k \in \mathcal{Z}^d} \exp(-\|\xi + 2\pi k\|^2/4\lambda), \quad \xi \in \mathcal{R}^d. \quad (2.9)$$

Finally, the decay of the Gaussian ensures that σ is continuous, being a uniformly convergent sum of continuous functions.

This result is of little use unless we know the minimum and maximum values of the symbol function for the Gaussian. Therefore we show next that explicit expressions for these numbers may be calculated from properties of Theta functions. Lemmata 2.7 and 2.8 address the cases when d = 1 and $d \ge 1$, respectively.

Lemma 2.7. Let λ be a positive constant and let E_1 : $\mathcal{R} \to \mathcal{R}$ be the 2π -periodic function

$$E_{1}(t) = \sum_{k=-\infty}^{\infty} \exp(-\lambda(t+2k\pi)^{2}).$$

Then $E_1(0) \ge E_1(t) \ge E_1(\pi)$ for all $t \in \mathcal{R}$.

Proof. An application of the Poisson summation formula provides the relation

$$E_{1}(t) = (4\pi\lambda)^{-1/2} \sum_{k=-\infty}^{\infty} e^{-k^{2}/4\lambda} e^{ikt}$$
$$= (4\pi\lambda)^{-1/2} \left(1 + 2 \sum_{k=1}^{\infty} e^{-k^{2}/4\lambda} \cos(kt) \right).$$

This is a Theta function. Indeed, using the notation of Whittaker and Watson [11, Sect. 21.11], it is a Theta function of Jacobi type

$$\vartheta_3(z,q) = 1 + 2 \sum_{k=1}^{\infty} q^{k^2} \cos(2kz),$$

where $q \in \mathcal{C}$ and |q| < 1. Choosing $q = e^{-1/4\lambda}$, we obtain the relation

$$E_1(t) = (4\pi\lambda)^{-1/2} \vartheta_3(t/2, q).$$

The useful product formula

$$\vartheta_3(z,q) = G \prod_{k=1}^{\infty} (1 + 2q^{2k-1} \cos 2z + q^{4k-2}),$$

where $G = \prod_{k=1}^{\infty} (1 - q^{2k})$, is given in Whittaker and Watson [11, Sect. 21.3 and 21.42]. Thus

$$E_1(t) = (4\pi\lambda)^{-1/2} G \prod_{k=1}^{\infty} (1 + 2q^{2k-1} \cos t + q^{4k-2}), \qquad t \in \mathcal{R}.$$

Now each term of the infinite product is a decreasing function on the interval $[0, \pi]$, which implies that E_1 is a decreasing function on $[0, \pi]$.

Since E_1 is an even 2π -periodic function, we deduce that E_1 attains its global minimum at $t = \pi$ and its maximum at t = 0.

Lemma 2.8. Let λ be a positive constant and let E_d : $\mathcal{R}^d \to \mathcal{R}^d$ be the $[0, 2\pi]^d$ -periodic function given by

$$E_d(x) = \sum_{k \in \mathcal{Z}^d} \exp(-\lambda \|t + 2k\pi\|^2), \qquad t = (t_1, \dots, t_d) \in \mathcal{R}^d.$$

Then $E_d(0) \ge E_d(t) \ge E_d(\pi e)$, where $e = [1, 1, ..., 1]^T$.

Proof. The key observation is the equation

$$E_d(t) = \prod_{k=1}^d E_1(t_k).$$

Thus $E_d(0) = \prod_{k=1}^d E_1(0) \ge \prod_{k=1}^d E_1(t_k) = E_d(t) \ge \prod_{k=1}^d E_1(\pi) = E_d(\pi e)$, using the previous lemma.

These lemmata imply that in the Gaussian case the maximum and minimum values of the symbol function occur at t = 0 and $t = \pi e$, respectively, where $e = [1, ..., 1]^T$. Therefore we deduce from formula (2.9) that the constants of Proposition 2.4 are the expressions

$$m = (\pi/\lambda)^{d/2} \sum_{k \in \mathcal{Z}^d} \exp(-\|\pi e + 2\pi k\|^2/4\lambda) \quad \text{and}$$

$$M = (\pi/\lambda)^{d/2} \sum_{k \in \mathcal{Z}^d} \exp(-\|\pi k\|^2/\lambda). \quad (2.10)$$

3. Conditionally Negative Definite Functions of Order 1

In this section we derive the optimal lower bound on the eigenvalue moduli of the distance matrices generated by the integers for a class of functions including the Hardy multiquadric.

DEFINITION 3.1. A real sequence $(y_j)_{\mathcal{Z}^d}$ is said to be zero-summing if it is finitely supported and $\sum_{j \in \mathcal{Z}^d} y_j = 0$.

Let $\varphi: [0, \infty) \to \mathcal{R}$ be a continuous function of algebraic growth. Thus it is meaningful to speak of the generalized Fourier transform of the radially symmetric function $\{\varphi(\|x\|): x \in \mathcal{R}^d\}$. We denote this transform by $\{\hat{\varphi}(\|\xi\|): \xi \in \mathcal{R}^d\}$, so emphasizing that it is a radially symmetric distribution, but we

note that $\hat{\varphi}$ depends on d. We shall restrict attention to the collection of functions described below.

DEFINITION 3.2. A function $\varphi: [0, \infty) \to \mathcal{R}$ will be termed *admissible* if it is a continuous function of algebraic growth which satisfies the following conditions:

- 1. $\hat{\varphi}$ is a continuous function on $\mathcal{R}^d \setminus \{0\}$.
- 2. The limit $\lim_{\|\xi\| \to 0} \|\xi\|^{d+1} \hat{\varphi}(\|\xi\|)$ exists.
- 3. The integral $\int_{\{\|\xi\| \ge 1\}} |\hat{\varphi}(\|\xi\|)| d\xi$ exists.

We now address the analogue of Proposition 2.3 for an admissible function.

PROPOSITION 3.3. Let $\varphi: [0, \infty) \to \mathcal{R}$ be an admissible function and let $(y_j)_{\mathcal{Z}^d}$ be a zero-summing sequence. Then for any choice of points $(x_j)_{\mathcal{Z}^d}$ in \mathcal{R}^d we have the identity

$$\sum_{j,k\in\mathcal{Z}^d} y_j y_k \varphi(\|x_j - x_k\|) = (2\pi)^{-d} \int_{\mathcal{R}^d} \left| \sum_{j\in\mathcal{Z}^d} y_j \exp(ix_j \xi) \right|^2 \hat{\varphi}(\|\xi\|) d\xi.$$
(3.1)

Proof. Let $\hat{g}: \mathcal{R}^d \to \mathcal{R}$ be the function defined by

$$\hat{g}(\xi) = \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ix_j \xi) \right|^2 \varphi(\|\xi\|).$$

Then \hat{g} is an absolutely integrable function on \mathscr{R}^d , because of the conditions on φ and because $(y_j)_{\mathscr{L}^d}$ is a zero-summing sequence. Thus \hat{g} is the generalized transform of $\sum_{j,k} y_j y_k \varphi(\|\cdot + x_j - x_k\|)$, and by standard properties of generalized Fourier transforms we deduce that

$$\sum_{j,k} y_j y_k \varphi (\|x + x_j - x_k\|)$$

$$= (2\pi)^{-d} \int_{\mathscr{R}^d} \left| \sum_{j \in \mathscr{Z}^d} y_j \exp(ix_j \xi) \right|^2 \hat{\varphi}(\|\xi\|) \exp(ix \xi) d\xi.$$

The proof is completed by setting x = 0.

We come now to the subject that is given in the title of this section.

DEFINITION 3.4. Let $\varphi: [0, \infty) \to \mathcal{R}$ be a continuous function. We shall say that φ is *conditionally negative definite of order* 1 *on every* \mathcal{R}^d ,

hereafter shortened to CND1, if we have the inequality

$$\sum_{j,k \in \mathcal{Z}^d} y_j y_k \varphi(\|x_j - x_k\|) \le 0,$$

for every positive integer d, for every zero-summing sequence $(y_j)_{\mathcal{Z}^d}$ and for any choice of points $(x_j)_{\mathcal{Z}^d}$ in \mathcal{R}^d .

Such functions were completely characterized by Schoenberg [9].

THEOREM 3.5. A continuous function $\varphi: [0, \infty) \to \mathcal{R}$ is CND1 if and only if there exists a nondecreasing function $\alpha: [0, \infty) \to \mathcal{R}$ such that

$$\varphi(r) = \varphi(0) + \int_0^\infty [1 - \exp(-tr^2)] t^{-1} d\alpha(t), \quad \text{for } r > 0,$$

and the integral $\int_{1}^{\infty} t^{-1} d\alpha(t)$ exists.

Proof. This is Theorem 6 of Schoenberg [9].

Thus $d\alpha$ is a positive Borel measure such that

$$\int_0^1 d\alpha(t) < \infty \quad \text{and} \quad \int_1^\infty t^{-1} d\alpha(t) < \infty.$$

Further, it is a consequence of this theorem that there exist constants A and B such that $\varphi(r) \leq Ar^2 + B$, where A and B are constants. In order to prove this assertion, we note the elementary inequalities

$$\int_{1}^{\infty} \left[1 - \exp(-tr^{2})\right] t^{-1} d\alpha(t) \leq \int_{1}^{\infty} t^{-1} d\alpha(t) < \infty,$$

and

$$\int_0^1 [1 - \exp(-tr^2)] t^{-1} d\alpha(t) \le r^2 \int_0^1 d\alpha(t).$$

Thus $A = \alpha(1) - \alpha(0)$ and $B = \varphi(0) + \int_1^\infty t^{-1} d\alpha(t)$ suffice. Therefore we may regard a CND1 function as a tempered distribution and it possesses a generalized Fourier transform. The following relation between the transform and the integral representation of Theorem 3.5 will be essential to our needs.

THEOREM 3.6. Let $\varphi: [0, \infty) \to \mathcal{R}$ be an admissible CND1 function. For $\xi \in \mathcal{R}^d \setminus \{0\}$, we have the formula

$$\hat{\varphi}(\|\xi\|) = -\int_0^\infty \exp(-\|\xi\|^2/4t) (\pi/t)^{d/2} t^{-1} d\alpha(t). \tag{3.2}$$

Before embarking on the proof of this theorem, we require some groundwork. We shall say that a function $f: \mathcal{R}^d \setminus \{0\} \to \mathcal{R}$ is symmetric if f(-x) = f(x), for every $x \in \mathcal{R}^d \setminus \{0\}$.

LEMMA 3.7. Let $\alpha: [0, \infty) \to \mathcal{R}$ be a nondecreasing function such that the integral $\int_1^{\infty} t^{-1} d\alpha(t)$ exists. Then the function

$$\psi(\xi) = -\int_0^\infty \exp(-\|\xi\|^2/4t) (\pi/t)^{d/2} t^{-1} d\alpha(t), \qquad \xi \in \mathcal{R}^d \setminus \{0\},$$
(3.3)

is a symmetric smooth function, that is every derivative exists.

Proof. For every nonzero ξ , the limit

$$\lim_{t \to 0} \exp(-\|\xi\|^2/4t) (\pi/t)^{d/2} t^{-1} = 0$$

implies that the integrand of expression (3.3) is a continuous function on $[0, \infty)$. Therefore, it follows from the inequality

$$\int_{1}^{\infty} \exp(-\|\xi\|^{2}/4t) (\pi/t)^{d/2} t^{-1} d\alpha(t) \le \pi^{d/2} \int_{1}^{\infty} t^{-1} d\alpha(t) < \infty$$

that the integral is well-defined. Further, a similar argument for nonzero ξ shows that every derivative of the integrand with respect to ξ is also absolutely integrable for $t \in [0, \infty)$, which implies that every derivative of ψ exists. The proof is complete, the symmetry of ψ being obvious.

Lemma 3.8. Let $f: \mathcal{R}^d \to \mathcal{R}$ be a symmetric absolutely integrable function such that

$$\int_{\mathcal{R}^d} \left| \sum_{i \in \mathcal{T}^d} a_i \exp(ix_i t) \right|^2 f(t) dt = 0,$$

for every finitely supported sequence $(a_j)_{\mathcal{Z}^d}$ and for any choice of points $(x_i)_{\mathcal{Z}^d}$. Then f must vanish almost everywhere.

Proof. The given conditions on f imply that the Fourier transform \hat{f} is a symmetric function that satisfies the equation

$$\sum_{j,k\in\mathcal{Z}^d} a_j a_k \hat{f}(x_j - x_k) = 0,$$

for every finitely supported sequence $(a_j)_{\mathcal{L}^d}$ and for all points $(x_j)_{\mathcal{L}^d}$ in \mathcal{R}^d . Let l and m be different integers and let a_l and a_m be the only

nonzero elements of $(a_j)_{\mathcal{Z}^d}$. We now choose any point $\xi \in \mathcal{R}^d \setminus \{0\}$ and set $x_i = 0$, $x_m = \xi$, which provides the equation

$$\begin{pmatrix} a_l \\ a_m \end{pmatrix}^{\mathsf{T}} \begin{pmatrix} \hat{f}(0) & \hat{f}(\xi) \\ \hat{f}(\xi) & \hat{f}(0) \end{pmatrix} \begin{pmatrix} a_l \\ a_m \end{pmatrix} = 0, \quad \text{for all } a_l, a_m \in \mathcal{R}.$$

Therefore $\hat{f}(0) = \hat{f}(\xi) = 0$, and since ξ was arbitrary, \hat{f} can only be the zero function. Consequently f must vanish almost everywhere.

COROLLARY 3.9. Let $g: \mathcal{R}^d \setminus \{0\} \to \mathcal{R}$ be a symmetric continuous function such that

$$\int_{\mathscr{D}^d} \left| \sum_{j \in \mathscr{Z}^d} y_j \exp(ix_j \xi) \right|^2 |g(\xi)| d\xi < \infty$$
 (3.4)

and

$$\int_{\mathscr{R}^d} \left| \sum_{j \in \mathscr{Z}^d} y_j \exp(ix_j \xi) \right|^2 g(\xi) d\xi = 0, \tag{3.5}$$

for every zero-summing sequence $(y_j)_{\mathcal{Z}^d}$ and for any choice of points $(x_j)_{\mathcal{Z}^d}$. Then $g(\xi) = 0$ for every $\xi \in \mathcal{R}^d \setminus \{0\}$.

Proof. For any integer $k \in \{1, ..., d\}$ and for any positive real number λ , let h be the symmetric function

$$h(\xi) = g(\xi)\sin^2\lambda\xi_k$$
, $\xi \in \mathcal{R}^d \setminus \{0\}$.

The relation

$$h(\xi) = g(\xi) \left| \frac{1}{2} \exp(i\lambda \xi_k) - \frac{1}{2} \exp(-i\lambda \xi_k) \right|^2$$

and condition (3.4) imply that h is absolutely integrable.

Let $(a_j)_{\mathcal{Z}^d}$ be any real finitely supported sequence and let $(b_j)_{\mathcal{Z}^d}$ be any sequence of points in \mathcal{R}^d . We define a real sequence $(y_j)_{\mathcal{Z}^d}$ and points $(x_j)_{\mathcal{Z}^d}$ in \mathcal{R}^d by the equation

$$\sum_{j \in \mathcal{Z}^d} y_j \exp(ix_j \xi) = \sin \lambda \xi_k \sum_{j \in \mathcal{Z}^d} a_j \exp(ib_j \xi).$$

Thus $(y_j)_{\mathcal{Z}^d}$ is a sequence of finite support. Further, setting $\xi = 0$, we deduce that $\sum_{j \in \mathcal{Z}^d} y_j = 0$, so $(y_j)_{\mathcal{Z}^d}$ is a zero-summing sequence. By

condition (3.5), we have

$$0 = \int_{\mathcal{R}^d} \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ix_j \xi) \right|^2 g(\xi) \ d\xi = \int_{\mathcal{R}^d} \left| \sum_{j \in \mathcal{Z}^d} a_j \exp(ib_j \xi) \right|^2 h(\xi) \ d\xi.$$

Therefore we can apply Lemma 3.8 to h, finding that it vanishes almost everywhere. Hence the continuity of g for nonzero argument implies that $g(\xi)\sin^2\lambda\xi_k=0$ for $\xi\neq0$. But for every nonzero ξ there exist $k\in\{1,\ldots,d\}$ and $\lambda>0$ such that $\sin\lambda\xi_k\neq0$. Consequently g vanishes on $\mathscr{R}^d\setminus\{0\}$.

We now complete the proof of Theorem 3.6.

Proof of Theorem 3.6. Let $(y_j)_{\mathcal{Z}^d}$ be a zero-summing sequence and let $(x_j)_{\mathcal{Z}^d}$ be any set of points in \mathcal{R}^d . Then Theorem 3.5 provides the expression

$$\begin{split} &\sum_{j,k \in \mathcal{Z}^d} y_j y_k \varphi \big(\|x_j - x_k\| \big) \\ &= - \int_0^\infty \bigg(\sum_{j,k \in \mathcal{Z}^d} y_j y_k \exp \big(-t \|x_j - x_k\|^2 \big) \bigg) t^{-1} \, d\alpha(t), \end{split}$$

this integral being well-defined because of the condition $\sum_{j \in \mathcal{Z}^d} y_j = 0$. Therefore, using Proposition 2.3 with $f(\cdot) = \exp(-t\|\cdot\|^2)$ in order to restate the Gaussian quadratic form in the integrand, we find the equation

$$\sum_{j,k \in \mathcal{Z}^d} y_j y_k \varphi(\|x_j - x_k\|)$$

$$= -\int_0^\infty \left[(2\pi)^{-d} \int_{\mathcal{R}^d} \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ix_j \xi) \right|^2 (\pi/t)^{d/2} \right] \times \exp(-\|\xi\|^2 / 4t) d\xi d\xi$$

$$= (2\pi)^{-d} \int_{\Re^d} \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ix_j \xi) \right|^2 \psi(\xi) d\xi,$$

where we have used Fubini's theorem to exchange the order of integration and where ψ is the function defined in (3.3). By comparing this equation with the assertion of Proposition 3.3, we see that the difference $g(\xi) = \hat{\varphi}(||\xi||) - \psi(\xi)$ satisfies the conditions of Corollary 3.9. Hence $\hat{\varphi}(||\xi||) = \psi(\xi)$ for all $\xi \in \mathcal{R}^d \setminus \{0\}$. The proof is complete.

Remark. An immediate consequence of this theorem is that the generalized Fourier transform of an admissible CND1 function cannot change sign.

The appearance of the Gaussian quadratic form in the proof of Theorem 3.6 enables us to use the bounds of Lemma 2.8, which gives the following result.

THEOREM 3.10. Let $\varphi: [0, \infty) \to \mathcal{R}$ be an admissible CND1 function and let $(y_i)_{\mathcal{Z}^d}$ be a zero-summing sequence. Then we have the inequality

$$\left|\sum_{j,k\in\mathbb{Z}^d} y_j y_k \varphi(\|j-k\|)\right| \geq \left|\sigma(\pi e)\right| \sum_{j\in\mathbb{Z}^d} y_j^2,$$

where $e = [1, ..., 1]^{T}$.

Proof. Applying (3.1) and dissecting \mathcal{R}^d into integer translates of the cube $[0, 2\pi]^d$, we obtain the equations

$$\left| \sum_{j,k \in \mathcal{Z}^d} y_j y_k \varphi(\|j - k\|) \right| = (2\pi)^{-d} \int_{\mathcal{R}^d} \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ij\xi) \right|^2 |\hat{\varphi}(\|\xi\|)| d\xi$$

$$= (2\pi)^{-d} \int_{[0,2\pi]^d} \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ij\xi) \right|^2 |\sigma(\xi)| d\xi,$$
(3.6)

where the interchange of summation and integration is justified by Fubini's theorem, and where we have used the fact that $\hat{\varphi}$ does not change sign. Here the symbol function has the usual form (2.5). Further, using (3.2), we again apply Fubini's theorem to deduce the formula

$$\begin{aligned} |\sigma(\xi)| &= \sum_{k \in \mathcal{Z}^d} |\hat{\varphi}(\|\xi + 2\pi k\|)| \\ &= \int_0^\infty \left(\sum_{k \in \mathcal{Z}^d} \exp(-\|\xi + 2\pi k\|^2/4t) \right) (\pi/t)^{d/2} t^{-1} d\alpha(t). \end{aligned}$$

Then it follows from Lemma 2.8 that we have the bound

$$|\sigma(\xi)| \ge \int_0^\infty \left(\sum_{k \in \mathcal{Z}^d} \exp\left(-\|\pi e + 2\pi k\|^2 / 4t\right) \right) (\pi/t)^{d/2} t^{-1} d\alpha(t)$$

$$= |\sigma(\pi e)|. \tag{3.7}$$

The required inequality is now a consequence of (3.6) and the Parseval

relation

$$(2\pi)^{-d} \int_{[0,2\pi]^d} \left| \sum_{j \in \mathcal{Z}^d} y_j \exp(ij\xi) \right|^2 d\xi = \sum_{j \in \mathcal{Z}^d} y_j^2. \quad \blacksquare$$

When the symbol function is continuous on $\mathscr{R}^d \setminus 2\pi \mathscr{Z}^d$, we can show that the previous inequality is optimal using a modification of the proof of Proposition 2.5. Specifically, we construct a set $\{(y_j^{(n)})_{\mathscr{Z}^d}: n=1,2,\ldots\}$ of zero-summing sequences such that $\lim_{n\to\infty} \sum_{i\in\mathscr{Z}^d} (y_i^{(n)})^2 = 1$ and

$$\lim_{n\to\infty}\left|\sum_{j,k\in\mathbb{Z}^d}y_j^{(n)}y_k^{(n)}\varphi(\|j-k\|)\right|=\left|\sigma(\pi e)\right|,$$

which implies that we cannot replace $|\sigma(\pi e)|$ by any larger number in Theorem 3.10.

COROLLARY 3.11. Let $\varphi: [0, \infty) \to \mathcal{R}$ satisfy the conditions of Theorem 3.10 and let the symbol function be continuous in the set $\mathcal{R}^d \setminus 2\pi \mathcal{Z}^d$. Then the bound of Theorem 3.10 is optimal.

Proof. Let m be an integer such that $4m \ge d + 1$ and let S_m be the trigonometric polynomial

$$S_m(\xi) = \left[d^{-1} \sum_{j=1}^d \sin^2(\xi_j/2) \right]^{2m}, \quad \xi \in \mathcal{R}^d.$$

Recalling from Lemma 2.2 that the multivariate Fejér kernel is the square of the modulus of a trigonometric polynomial with real coefficients, we choose a finitely supported sequence $(y_j^{(n)})_{\mathbb{Z}^d}$ satisfying the equations

$$\left|\sum_{j\in\mathcal{Z}^d} y_j^{(n)} \exp(ij\xi)\right|^2 = K_n(\xi - \pi e) S_m(\xi), \qquad \xi \in \mathcal{R}^d. \tag{3.8}$$

Further, setting $\xi = 0$ we see that $(y_j^{(n)})_{\mathcal{Z}^d}$ is a zero-summing sequence. Applying (3.6), we find the relation

$$\left| \sum_{j,k \in \mathcal{Z}^d} y_j^{(n)} y_k^{(n)} \varphi(\|j - k\|) \right|$$

$$= (2\pi)^{-d} \int_{[0,2\pi]^d} K_n(\xi - \pi e) S_m(\xi) |\sigma(\xi)| d\xi. \tag{3.9}$$

Moreover, because the second condition of Definition 3.2 implies that

 $S_m[\sigma]$ is a continuous function, Lemma 2.2 provides the equations

$$\lim_{n\to\infty} (2\pi)^{-d} \int_{[0,2\pi]^d} K_n(\xi - \pi e) S_m(\xi) |\sigma(\xi)| d\xi$$
$$= S_m(\pi e) |\sigma(\pi e)| = |\sigma(\pi e)|.$$

It follows from (3.9) that we have the limit

$$\lim_{n\to\infty}\left|\sum_{j,k\in\mathbb{Z}^d}y_j^{(n)}y_k^{(n)}\varphi(\|j-k\|)\right|=\left|\sigma(\pi e)\right|.$$

Finally, since S_m is a continuous function, another application of Lemma 2.2 yields the equation

$$\lim_{n\to\infty} (2\pi)^{-d} \int_{[0,2\pi]^d} K_n(\xi-\pi e) S_m(\xi) d\xi = S_m(\pi e) = 1.$$

By substituting expression (3.8) into the left-hand side and employing the Parseval relation

$$(2\pi)^{-d} \int_{[0,2\pi]^d} \left| \sum_{j \in \mathcal{Z}^d} y_j^{(n)} \exp(ij\xi) \right|^2 d\xi = \sum_{j \in \mathcal{Z}^d} \left(y_j^{(n)} \right)^2$$

we find the relation $\lim_{n\to\infty}\sum_{i\in\mathcal{Z}^d}(y_i^{(n)})^2=1$.

4. Applications

This section relates the optimal inequality given in Theorem 3.10 to the spectrum of the distance matrix, using an approach due to Ball [2]. We apply the following theorem.

THEOREM 4.1. Let $A \in \mathcal{R}^{n \times n}$ be a symmetric matrix with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let E be any subspace of \mathcal{R}^n of dimension m. Then we have the inequality

$$\max\{x^{T}Ax : x^{T}x = 1, x \perp E\} \ge \lambda_{m+1}$$

Proof. This is the Courant-Fischer minimax theorem. See Wilkinson [12, p. 99ff]. ■

For any finite subset N of \mathcal{Z}^d , let A_N be the distance matrix $(\varphi(\|j-k\|))_{j,k\in N}$. Further, let the eigenvalues of A_N be $\lambda_1 \geq \cdots \geq \lambda_{|N|}$, where |N| is the cardinality of N, and let λ_{\min}^N be the smallest eigenvalue in modulus.

PROPOSITION 4.2. Let $\varphi: [0, \infty) \to \mathcal{R}$ be a CND1 function that is not identically zero. Let $\varphi(0) \ge 0$ and let μ be a positive constant such that

$$\sum_{j,k\in\mathcal{Z}^d} y_j y_k \varphi(\|j-k\|) \le -\mu \sum_{j\in\mathcal{Z}^d} y_j^2, \tag{4.1}$$

for every zero-summing sequence $(y_j)_{\mathcal{Z}^d}$. Then for every finite subset N of \mathcal{Z}^d we have the bound

$$\left|\lambda_{\min}^{N}\right| \geq \mu$$
.

Proof. Equation (4.1) implies that

$$y^{\mathrm{T}}A_{N}y \leq -\mu y^{\mathrm{T}}y,$$

for every vector $(y_j)_{j\in N}$ such that $\sum_{j\in N}y_j=0$. Thus, Theorem 4.1 implies that the eigenvalues of A_N satisfy $-\mu \geq \lambda_2 \geq \cdots \geq \lambda_{|N|}$, where the subspace E of that theorem is simply the span of the vector $[1,1,\ldots,1]^T\in \mathscr{R}^N$. In particular, $0>\lambda_2\geq \cdots \geq \lambda_{|N|}$. This observation and the condition $\varphi(0)\geq 0$ provide the expressions

$$0 \le \operatorname{trace} A_N = \lambda_1 + \sum_{j=2}^{|N|} \lambda_j = \lambda_1 - \sum_{j=2}^{|N|} |\lambda_j|.$$

Hence we have the relations $\lambda_{\min}^N = \lambda_2 \le -\mu$. The proof is complete.

We now turn to the case of the multiquadric $\varphi_c(r) = (r^2 + c^2)^{1/2}$, in order to furnish a practical example of the above theory. This is a non-negative CND1 function (see Micchelli [6]) and its generalized Fourier transform is the expression

$$\hat{\varphi}_{c}(\|\xi\|) = -\pi^{-1} (2\pi c/\|\xi\|)^{(d+1)/2} K_{(d+1)/2}(c\|\xi\|),$$

for nonzero ξ , which may be found in Jones [4]. Here $\{K_{\nu}(r): r > 0\}$ is a modified Bessel function which is positive and smooth in \mathcal{R}^+ , has a pole at the origin, and decays exponentially (Abramowitz and Stegun [1]). Consequently, φ_c is a non-negative admissible CND1 function. Further, the exponential decay of $\hat{\varphi}_c$ ensures that the symbol function

$$\sigma_c(\xi) = \sum_{k \in \mathcal{Z}^d} \hat{\varphi}_c(\|\xi + 2\pi k\|) \tag{4.2}$$

is continuous for $\xi \in \mathcal{R}^d \setminus 2\pi \mathcal{Z}^d$. Therefore, given any finite subset N of

 \mathcal{Z}^d , Theorem 3.10 and Proposition 4.2 imply that the distance matrix A_N has every eigenvalue bounded away from zero by at least

$$\mu_c = \sum_{k \in \mathcal{Z}^d} |\hat{\varphi}_c(\|\pi e + 2\pi k\|)|, \tag{4.3}$$

where $e = [1, 1, ..., 1]^T \in \mathcal{R}^d$. Moreover, Corollary 3.11 shows that this bound is optimal.

It follows from (4.3) that $\mu_c \to 0$ as $c \to \infty$, because of the exponential decay of the modified Bessel functions for large argument. For example, in the univariate case we have the formula

$$\mu_c = (4c/\pi)[K_1(c\pi) + K_1(3c\pi)/3 + K_1(5c\pi)/5 + \cdots],$$

and Table I displays some values of μ_c . Of course, a practical implication of this result is that we cannot expect accurate direct solution of the interpolation equations for even quite modest values of c, at least without using some special technique.

The optimal bound is achieved only when the number of centres is infinite. Therefore it is interesting to investigate how rapidly $|\lambda_{\min}^N|$ converges to the optimal lower bound as |N| increases. Table II displays $|\lambda_{\min}^N| = \mu_c(n)$, say, for the distance matrix $(\varphi_c(||j-k||))_{j,k=0}^{n-1}$ for several values of n when c=1. The third column lists close estimates of $\mu_c(n)$ obtained using a theorem of Szegő (see Sect. 5.2 of Grenander and Szegő [5]). Specifically, Szegő's theorem provides the approximation

$$\mu_c(n) \approx \sigma_c(\pi + \pi/n),$$

where σ_c is the function defined in (4.2). This theorem of Szegő requires the fact that the minimum value of the symbol function is attained at π ,

TABLE 1 The Optimal Bound on the Smallest Eigenvalue as $c \to \infty$

c	Optimal bound
1.0	4.319455×10^{-2}
2.0	2.513366×10^{-3}
3.0	1.306969×10^{-4}
4.0	6.462443×10^{-6}
5.0	3.104941×10^{-7}
10.0	6.542373×10^{-14}
15.0	2.089078×10^{-20}

n	$\mu_1(n)$	$\sigma_{\parallel}(\pi + \pi/n)$
100	4.324685×10^{-2}	4.324653×10^{-2}
150	4.321774×10^{-2}	4.321765×10^{-2}
200	4.320758×10^{-2}	4.320754×10^{-2}
250	4.320288×10^{-2}	4.320286×10^{-2}
300	4.320033×10^{-2}	4.320032×10^{-2}
350	4.319880×10^{-2}	4.319879×10^{-2}

TABLE II Some Calculated and Estimated Values of λ_{\min}^N when c=1

which is inequality (3.7). Further, it provides the estimates

$$\lambda_{k+1} \approx \sigma_c(\pi + k\pi/n), \qquad k = 1, \ldots, n-1,$$

for all the negative eigenvalues of the distance matrix. Figure 1 displays the numbers $\{-1/\lambda_k: k=2,\ldots,n\}$ and their estimates $\{-1/\sigma(\pi+k\pi/n): k=1,\ldots,n-1\}$ in the case when n=100. We see that the agreement is excellent. Furthermore, this modification of the classical theory of Toeplitz forms also provides an interesting and useful perspective on the construction of efficient preconditioners for the conjugate gradient solution of the interpolation equations. We include no further

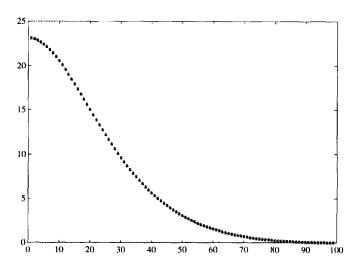


Fig. 1. Spectral estimates for a distance matrix of order 100. Key: (+) calculated; (\times) estimated.

information on these topics, this last paragraph being presented as an apéritif to the paper of Baxter [3].

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