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Conditions for bound states in a periodic linear chain, and the spectra of a class of Toeplitz operators in terms of polylogarithm functions

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Abstract

Conditions for bound states for a periodic linear chain are given within the framework of an exactly solvable non-relativistic quantum-mechanical model in three-dimensional space. These conditions express the strength parameter in terms of the distance between two consecutive centres of the chain, and of the range interaction parameter. This expression can be formulated in terms of polylogarithm functions, and, in some particular cases, in terms of the Riemann zeta function. An interesting mathematical result is that these expressions also correspond to the spectra of Toeplitz complex symmetric operators. The non-trivial zeros of the Riemann zeta function are interpreted as multiple points, at the origin, of the spectra of these Toeplitz operators.

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1. Introduction

Solvable models in quantum mechanics are extremely useful, both for obtaining specific results and for testing different methods of approximation which are required for studying non-exactly solvable models. Few solvable models exist, and among them, models based on the so-called 'point interactions, zero-range potentials, delta interactions, Fermi pseudopotentials, ...' have been thoroughly studied and applied (see e.g. [1, 2]).

Recently, another solvable model with non-zero range has been proposed [3], and applied [4–6]. The (one-particle) Hamiltonian for this model is [3]: $H = \frac{p^2}{2M} + \sum_{j=1}^{n} V_j$, where V_j is a sum of separable interactions centred on the point P_j determined with respect to an arbitrary origin O by the vector $\mathbf{a}_j = \vec{OP_j}$. Specifically

$$V_j = \sum_k \lambda_j^k \left|\xi_j^k\right\rangle\left\langle\xi_j^k\right|$$

$$\left|\xi_j^k\right\rangle = \exp(-\mathrm{i}\mathbf{a}_j\cdot\mathbf{p})\left(r_j^k\right)^{3/2}\left|r_j^k, \ell_j^k, m_j^k\right\rangle$$

where $\mathbf{p}$ is the momentum operator. The vector $\left|r_j^k, \ell_j^k, m_j^k\right\rangle$ is an eigenvector of the squared orbital angular momentum with eigenvalue $\ell_j^k\left(\ell_j^k+1\right)$, an eigenvector of the component ℓ_z of the orbital angular momentum with eigenvalue m_j^k, and a generalized eigenvector of the radial position operator with generalized eigenvalue r_j^k,

$$(\ell_x \pm \mathrm{i}\ell_y)|r,\ell,m\rangle = \sqrt{(\ell \pm m+1)(\ell \mp m)}|r,\ell,m\pm 1\rangle$$

$$\langle r',\ell',m' \mid r,\ell,m\rangle = \frac{\delta(r'-r)}{r^2}\delta_{\ell\ell'}\delta_{mm'}$$

$$\langle \mathbf{r}' \mid r,\ell,m\rangle = \frac{\delta(r'-r)}{r^2} Y_\ell^m\left(\frac{\mathbf{r}'}{r}\right).$$

The operator $\exp(-\mathrm{i}\mathbf{a}_j\cdot\mathbf{p})$ translates the vector $\left|r_j^k, \ell_j^k, m_j^k\right\rangle$ from the point O to the point P_j. The parameters r_j^k and λ_j^k are respectively the range and the strength of the separable interaction $\left|\xi_j^k\right\rangle\left\langle\xi_j^k\right|$. For more details, see [3].

In the present paper, we consider a linear periodic configuration $\mathbf{a}_j = j\mathbf{L}$ with $j = -\infty, \ldots, -2, -1, 0, 1, 2, \ldots, \infty$ and $\mathbf{L}$ an arbitrary constant vector which determines the Oz axis. We also consider only one value for the strength, range parameters, and the orbital quantum numbers: $\lambda_j^k = \lambda, r_j^k = r, \ell_j^k = \ell$. The Hamiltonian thus becomes

$$H_\ell^m = \lim_{K\to\infty} {}_{2K+1}H_\ell^m \tag{1}$$

$$_{2K+1}H_\ell^m = \frac{p^2}{2M} + \lambda \sum_{j=-K}^{K} |\xi_j\rangle\langle\xi_j| \tag{2}$$

$$|\xi_j\rangle = \exp(-\mathrm{i}j\mathbf{L}\cdot\mathbf{p})r^{3/2}|r,\ell,m\rangle. \tag{3}$$

The projection of the orbital angular momentum, $\left(m_j^k = m\right)$, is a good quantum number because the operator ℓ_z commutes with H_ℓ^m and $_{2K+1}H_\ell^m$. Mirror reflection through a plane containing the chain axis is a symmetry operation which changes m into $-m$. As a result, the energy eigenvalues depend on $|m|$ only.

The restriction to only one value of orbital quantum number ℓ may first appear unphysical. This restriction is however physical in the low-energy limit where only the partial wave $\ell = 0$ contributes, or for example, for alkali atoms in the ground state where only the partial wave $\ell = 1$ contributes.

In equation (2), the subscript $2K+1$ before H gives the number N of projectors in the right-hand side, when j varies between $-K$ and K. When $N \to \infty$, one therefore has a *doubly* infinite chain. In the study of a finite chain, we shall not restrict the problem to odd number of centres, and, from now on, $_N H_\ell^m = \frac{p^2}{2M} + \lambda\sum_{j=1}^N |\xi_j\rangle\langle\xi_j|$ will denote the Hamiltonian for a linear chain with N equidistant centres. The number of bound states of $_N H_\ell^m$ will be denoted by N_b. It will be seen in section 4.1 that $_N H_\ell^m$ has at most N bound states.

The physical question at the origin of the present work is: what are the conditions on the strength parameter λ, the range parameter r and the intercentre distance L, for having $\lim_{N\to\infty}\frac{N_b}{N} = \rho$ $(0 \leqslant \rho \leqslant 1)$? The answer will be given in section 4.2.1, equation (17).

In studying this problem, we are led to consider the (doubly) infinite *complex symmetric* Toeplitz matrix (i.e. a complex symmetric matrix whose elements are constant along each diagonal parallel to the main diagonal) $T(s)$:

$$\begin{array}{cccccc} \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & 2^{-s} & 3^{-s} & \dots \\ \dots & 1 & 0 & 1 & 2^{-s} & \dots \\ \dots & 2^{-s} & 1 & 0 & 1 & \dots \\ \dots & 3^{-s} & 2^{-s} & 1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{array}$$

Specifically,

$$-\infty \leqslant i, j \leqslant \infty \qquad \text{and} \qquad T_{ij}(s) = \begin{cases} 0 & \text{if } i = j \\ 1/|i-j|^s & \text{if } i \neq j \end{cases} \tag{4}$$

where i and j are elements of $\mathbb{Z}$, the set of relative integers, and where s is an arbitrary complex number. The spectrum $S(s)$ of $T(s)$ is given by

$$S(s) = \left\{ 2 \sum_{n=1}^{\infty} \frac{\cos(n\pi\beta)}{n^s} \;\middle|\; 0 \leqslant \beta \leqslant 1 \right\}$$

when this series converges and by an analytic continuation in terms of polylogarithm functions in the general case. This result is derived in section 5 for $s = 2\ell + 1$ ($\ell = 0, 1, 2, \dots$) and its extension to the case of more general s values is discussed in section 6. For $\ell > 0$, this result is a particular case of a general theorem concerning the spectrum of Toeplitz operators whose symbols (i.e. the functions whose Fourier coefficients a_n are given by the matrix element $a_{i-j} = T_{ij}$) belong to the functions space L^∞ on the circle (see e.g. theorem 1.2 of [7]). However, this general theorem does not concern the case $\ell = 0$ because in that case the symbol (given by the right-hand side of equation (18)) does not belong to L^∞. Anyway, the derivation of this result presented in section 5, valid for both cases $\ell = 0$ and $\ell \neq 0$, makes clear that β is the coordinate of a point in the reduced Brillouin zone, and therefore that the density of states at a point of the spectrum $S(s)$ of $T(s)$, characterized by β, corresponds to a uniform density in the variable β.

Finally, the zeros of the Riemann zeta function in the critical band $0 < \mathrm{Re}(s) < 1$ are interpreted as the s values for which the curve $S(s)$ in the complex plane has a multiple point at the origin, of multiplicity equal to four at least.

A necessary preliminary step before coming to these results is the determination, for fixed values of ℓ, m, of the relation between the strength λ, the range r and the intercentre distance L, for the existence of a zero-energy bound state (or resonance). This is the subject of the two following sections where both the cases of a finite and of an infinite linear chain are considered.

2. Zero energy for a finite linear chain

As explained in [3–6], the bound state energies for a finite number of centres, or equivalently the poles on the negative real axis of the resolvent

$$G(z) = \left[z - p^2/(2M) - \sum_k V_k \right]^{-1}$$

can be determined as the negative z values for which the determinant of a matrix $b(z)$ of order equal to the number N of centres is zero. This matrix $b(z)$ is defined by its matrix elements

$$b_{ij}(z) = \delta_{ij} - \lambda \langle \xi_i | G_0(z) | \xi_j \rangle$$

where $G_0(z) = [z - p^2/(2M)]^{-1}$ is the free resolvent. The wavefunctions of these bound states are exponentially decreasing at infinity. The diagonal elements of G_0 are given by (see equation (42) of [3])

$$(g_0)_{jj}(z) \equiv \langle \xi_j | G_0(z) | \xi_j \rangle = -2Mr^3 p h_\ell^+(pr) j_\ell(pr).$$

The non-diagonal elements of G_0 are given by (see equation (45) of [3])

$$(g_0)_{jn}(z) = -(-1)^m r^3 8\pi M p\, [j_\ell(pr)]^2\, (2\ell+1) \sqrt{\frac{1}{4\pi}} \sum_{\nu=0}^{2\ell} \sqrt{2\nu+1}\, \mathrm{i}^\nu$$
$$h_\nu^+(p|j-n|\,|\mathbf{L}|) Y_\nu^0(\overrightarrow{(j-n)\,\mathbf{L}}) \begin{pmatrix} l & l & \nu \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l & \nu \\ -m & m & 0 \end{pmatrix}$$

with $p \equiv \sqrt{2Mz}$. The right arrow in the argument of the spherical harmonics Y_ν^0 means a unit vector $\left(\overrightarrow{\mathbf{v}} \equiv \frac{\mathbf{v}}{|\mathbf{v}|}\right)$. The three j symbols are defined as in [8], and the spherical Bessel functions j_ℓ, h_ν^+, as in [9].

Let us consider the zero-energy case: $j_\ell(z) \sim \frac{z^\ell}{(2\ell+1)!!}$ and $h_\nu^+(z) \sim \frac{(2\nu-1)!!}{z^{\nu+1}}$ as $z \to 0$. In this limit, the diagonal matrix element is given by

$$\langle \xi_j | G_0(0) | \xi_j \rangle = -\frac{2Mr^2}{2\ell+1}. \tag{5}$$

For the non-diagonal matrix elements, one sees that only the term $\nu = 2\ell$ contributes in this limit. The polar angle in the spherical harmonics is 0 or π for the geometrical configuration of a linear chain on the z-axis. Since [8]

$$Y_{2\ell}^0(0,\varphi) = Y_{2\ell}^0(\pi,\varphi) = \sqrt{\frac{4\ell+1}{4\pi}}$$

and since [8]

$$(-1)^{j_2-j_1} \begin{pmatrix} j_1 & j_2 & j_1+j_2 \\ -m & m & 0 \end{pmatrix}$$
$$= \left[\frac{(2j_1)!\,(2j_2)!}{(2j_1+2j_2+1)!\,(j_1-m)!\,(j_1+m)!\,(j_2+m)!\,(j_2-m)!} \right]^{\frac{1}{2}} (j_1+j_2)!$$

one finally obtains

$$\langle \xi_j | G_0(0) | \xi_n \rangle = -\frac{2Mr^2}{(2\ell+1)} (-1)^{\ell+m} \left(\frac{r}{|j-n| L} \right)^{2\ell+1} \frac{(2\ell)!}{(l-m)!\,(l+m)!}.$$

Let us call λ_k the zeros (with respect to the variable λ) of the determinant of the matrix whose elements are $b_{ij}(0)$. Let us also introduce the symmetric Toeplitz matrix $T_N(2\ell+1)$ of order N:

$$1 \leqslant i, j \leqslant N \qquad \text{and} \qquad (T_N)_{ij}(s) = \begin{cases} 0 & \text{if } i = j \\ \frac{1}{|i-j|^s} & \text{if } i \neq j \end{cases}. \tag{6}$$

A short calculation shows that λ_k will be expressed in terms of the eigenvalues t_k of the real symmetric Toeplitz matrix $T_{2K+1}(2\ell+1)$ of order $2K+1$, by the relation

$$\frac{1}{\lambda_k} = -\frac{2Mr^2}{(2\ell+1)} \left[1 + g_\ell^m(\alpha)\, t_k \right] \tag{7}$$

$$g_\ell^m(\alpha) \equiv (-1)^{\ell+m} \frac{(2\ell)!}{(\ell-m)!\,(\ell+m)!} \alpha^{2\ell+1} \tag{8}$$

where from now on α is defined by

$$\alpha \equiv \frac{r}{L}. \tag{9}$$

One notes that

$$g_\ell^m(\alpha) = g_\ell^{-m}(\alpha) \tag{10}$$

as expected since the energy depends only on $|m|$ by mirror symmetry in a plane containing the chain axis.

It is recalled that $0 < \alpha \leqslant \frac{1}{2}$ since the distance L between two centres was supposed to be greater than twice the range r of the interactions in [3]. These finite real symmetric Toeplitz matrices clearly have zero trace.

3. Zero energy for infinite linear chain

The *first key point* of this paper is to note that for a (doubly) infinite linear chain, the problem is invariant by translation in the z-direction by integer multiples of L. The translation group is Abelian and its irreducible unitary representations are one dimensional. These irreducible representations can be characterized by a real number β. The energies of a single electron in an effective periodic interaction are thus indexed by a vector $\mathbf{k}$ in the first Brillouin zone of the reciprocal lattice (here $\mathbf{k} = \beta\frac{\pi}{L}\overrightarrow{\mathbf{z}}$, $-1 \leqslant \beta < 1$). This is the main result of what is known as the 'Bloch theorem' for periodic systems. Time reversal symmetry (which corresponds here to complex conjugation) yields [10] $E(-\mathbf{k}) = E(\mathbf{k})$, and thus, allows us to restrict the study to the reduced Brillouin zone corresponding to $0 \leqslant \beta \leqslant 1$. As is well known (see e.g. [11]), the determination of energy values of one electron for the case of an infinite number of centres on a lattice is reduced to the solution of the Schrödinger equation for a *single centre*, with periodic boundary conditions depending on $\mathbf{k}$. These boundary conditions relevant to the present case are periodic boundary conditions in the z-direction, and, for negative energy, an exponentially decreasing solution in the two other directions. It is then easy to see that the poles of the total resolvent $G_\beta(z)$ are solutions of

$$\frac{1}{\lambda} - \langle\xi|G_{0\beta}(z)|\xi\rangle = 0$$

(the index j of ξ_j is omitted as these diagonal elements are j independent). One then proceeds as in [4] and obtains

$$r^3\langle r, \ell, m|G_{0\beta}(0)|r, \ell, m\rangle = \frac{r^3}{(2\pi)^2}\frac{1}{L}\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}p_x\int_{-\infty}^{\infty}\mathrm{d}p_y(4\pi)^2\frac{|j_\ell(pr)|^2\left|Y_\ell^m(\overrightarrow{\mathbf{p}})\right|^2}{-p^2/2M}$$

$$p = \sqrt{p_x^2 + p_y^2 + \left[\frac{\pi}{L}(2n+\beta)\right]^2}.$$

The square modulus $\left|Y_\ell^m(\overrightarrow{\mathbf{p}})\right|^2$ is given by [8]

$$\left|Y_\ell^m(\overrightarrow{\mathbf{p}})\right|^2 = \frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}\left|P_\ell^m(\cos(\theta))\right|^2$$

$$\cos(\theta) = \frac{b_n}{\sqrt{p_x^2 + p_y^2 + b_n^2}}$$

$$b_n = \frac{\pi}{L}(2n+\beta)$$

where P_ℓ^m is an associated Legendre polynomial. The integral over $\mathrm{d}p_x\,\mathrm{d}p_y$ can be expressed in plane polar coordinates as $2\pi\int_0^\infty \sigma\,\mathrm{d}\sigma$ with $\left(p_x^2+p_y^2\right)=\sigma^2$. Finally, with the further change of variable $x=rp=r\sqrt{\sigma^2+b_n^2}$, one obtains

$$r^3\langle r,\ell,m|G_{0\beta}(0)|r,\ell,m\rangle=-4Mr^2\alpha\frac{(2\ell+1)\,(\ell-m)!}{(\ell+m)!}\sum_{n=-\infty}^{\infty}\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{\mathrm{d}x}{x}\,|j_\ell(x)|^2\left|P_\ell^m\left(\frac{(2n+\beta)\,\pi\alpha}{x}\right)\right|^2$$

where α is defined by equation (9). It is shown in appendix A how the sum $A_\ell^m(\alpha,\beta)$ of the series of integrals defined by

$$A_\ell^m(\alpha,\beta)\equiv\sum_{n=-\infty}^{\infty}\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{\mathrm{d}x}{x}\left|j_\ell(x)\,P_\ell^m\left(\frac{(2n+\beta)\,\pi\alpha}{x}\right)\right|^2 \tag{11}$$

can be evaluated (see equation (A.4)). The result given by equation (A.4) is *the second key point* of this paper. As a result, the critical values λ_c of λ are given by

$$\frac{1}{\lambda_c}=\langle\xi|G_{0\beta}(0)|\xi\rangle \tag{12}$$

$$=-\frac{2Mr^2}{(2\ell+1)}\left\{1+g_\ell^m(\alpha)\,2\sum_{j=1}^{\infty}\frac{\cos(j\pi\beta)}{j^{2\ell+1}}\right\} \tag{13}$$

where the function g_ℓ^m is defined by equation (8).

For $\alpha\to 0^+$, i.e. in the limit of infinite intercentre distances L, equation (13) reduces to the result given by equation (5) for one centre, provided the series $2\sum_{j=1}^{\infty}\cos(j\pi\beta)j^{-(2\ell+1)}$ converges. This series converges for every ℓ value $(0,1,2,\ldots)$ and for every β value in the interval [0, 1], except for the single case $\ell=0$ *and* $\beta=0$, where it has a logarithmic divergence.

4. Physical results

4.1. Maximal number of bound state of ${}_NH$

Application of the Hellmann–Feynman theorem $\frac{\partial E}{\partial\lambda}=\langle\Psi|\frac{\partial H}{\partial\lambda}|\Psi\rangle$ (see e.g. [12]) to the Hamiltonian ${}_NH=\frac{p^2}{2M}+\lambda\sum_{j=1}^{N}|\xi_j\rangle\langle\xi_j|$ gives

$$\frac{\partial E}{\partial\lambda}=\sum_{j=1}^{N}|\langle\Psi\mid\xi_j\rangle|^2$$

where E is an eigenvalue and $|\Psi\rangle$ a corresponding normalized eigenvector. One therefore deduces that the energies of the bound states are increasing functions of the real strength parameter λ. Let us first consider the Hamiltonian ${}_1H$ with one projector only. Then, it is easy to show that at most one bound state can exist (see e.g. [13]). More precisely, one bound state exists if $\lambda<-\frac{2\ell+1}{2Mr^2}={}_1\lambda$ (see equation (5)). Now let us consider the Hamiltonian ${}_2H$ with two projectors. The interlacing eigenvalue theorem for bordered Hermitian matrices (see e.g. [14]) shows that the eigenvalues $1/({}_2\lambda_i)$ $(i=1,2,{}_2\lambda_2<{}_2\lambda_1)$ of the matrix of order two, with elements $\langle\xi_i|G_0(0)|\xi_j\rangle$, will interlace ${}_1\lambda$. One deduces that one bound state exists if ${}_2\lambda_2<\lambda<{}_2\lambda_1$ and two bound states exist if $\lambda<{}_2\lambda_2$. A recursion over the number N of projectors finally shows that:

(i) There are at most N bound states for ${}_N H$.

(ii) The critical values ${}_N\lambda_k$ for which a zero-energy state exists for an Hamiltonian with N projectors interlace the critical values ${}_{N-1}\lambda_k$ for an Hamiltonian with $N-1$ projectors.

These results are general and do not depend on the particular nature of the states $|\xi_j\rangle$.

4.2. Proportion of bound states for an infinite chain

4.2.1. The general case. From now on, we define the function f by

$$f(s,\beta) \equiv 2\sum_{j=1}^{\infty} \frac{\cos(j\pi\beta)}{j^s} \tag{14}$$

when the series (14) converges, and otherwise by an analytic continuation, conveniently expressed in terms of the usual polylogarithm function Li_s (see equations (A.5), (A.6)),

$$f(s,\beta) = Li_s(\exp(\mathrm{i}\pi\beta)) + Li_s(\exp(-\mathrm{i}\pi\beta)). \tag{15}$$

For the five values $\beta = 0, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, 1$, the function $f(s,\beta)$ is simply related to the Riemann zeta function $\zeta(s)$:

$$f(s,0) = 2\zeta(s) \tag{16a}$$

$$f\left(s,\frac{1}{3}\right) = (1-2^{1-s})(1-3^{1-s})\zeta(s) \tag{16b}$$

$$f\left(s,\frac{1}{2}\right) = -2^{1-s}(1-2^{1-s})\zeta(s) \tag{16c}$$

$$f\left(s,\frac{2}{3}\right) = -(1-3^{1-s})\zeta(s) \tag{16d}$$

$$f(s,1) = -2(1-2^{1-s})\zeta(s). \tag{16e}$$

The function $f(2\ell+1,\beta)$ is a decreasing function of β for $0 \leqslant \beta \leqslant 1$. This can be seen from the Appell integral representation of the polylogarithm functions [15]

$$Li_s(z) = \frac{1}{\Gamma(s)}\int_0^{\infty} \frac{z t^{s-1}}{\exp(t)-z}\,\mathrm{d}t$$

which yields

$$f(s,\beta) = \frac{2}{\Gamma(s)}\int_0^{\infty} t^{s-1}\frac{\exp(t)\cos(\pi\beta)-1}{[\exp(t)-1]^2+2\exp(t)[1-\cos(\pi\beta)]}\,\mathrm{d}t.$$

For $s = 2\ell+1$, the integrand is real. Then, for $0 \leqslant \beta \leqslant 1$, the numerator and the denominator of the integrand are respectively decreasing and increasing functions of β, so that the integrand is a decreasing function of β, and therefore also is $f(2\ell+1,\beta)$, for every value of the orbital quantum number ℓ. Equations (13), (8) then show that two cases have to be distinguished according to the parity of $\ell \pm m$. If $\ell \pm m$ is even, λ_c is a decreasing function of β, whereas if $\ell \pm m$ is odd, λ_c is an increasing function of β. The proportion ρ of bound states of the Hamiltonian ${}_\infty H_\ell^m$, defined by $\rho = \lim_{N\to\infty}\frac{N_b}{N}$ for fixed values of the range parameter r, the internuclear distance L, will therefore depend on the value of the strength parameter λ according to the law

$$\frac{1}{\lambda} = \begin{cases} -\frac{2Mr^2}{(2\ell+1)}\left\{1+g_\ell^m(\alpha)f(2\ell+1,\rho)\right\} & \text{if } \ell \pm m \text{ even} \\ -\frac{2Mr^2}{(2\ell+1)}\left\{1+g_\ell^m(\alpha)f(2\ell+1,1-\rho)\right\} & \text{if } \ell \pm m \text{ odd.} \end{cases} \tag{17}$$

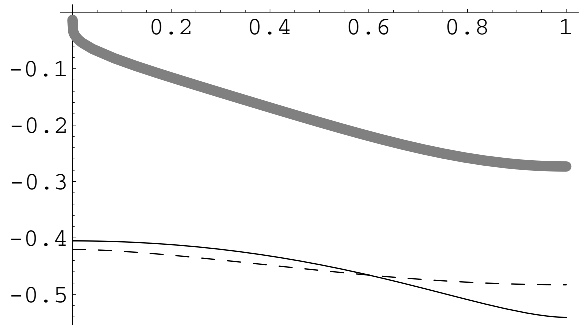


Figure 1. Infinite linear chain. λ (ordinate), as a function of ρ (abscissa), according to equation (17) (see the text). Thick grey curve: $\ell = |m| = 0$. Solid curve: $\ell = 1, |m| = 0$. Dashed curve: $\ell = 1, |m| = 1$.

For $\ell \pm m$ odd, the terms $\cos(j\pi(1-\rho))$ in the series defining $f(2\ell+1, 1-\rho)$ can also be written as $(-1)^j \cos(j\pi\rho)$. Figure 1 displays λ as a function of ρ for $\ell = m = 0$, and for $\ell = 1, |m| = 0, 1$ according to equation (17). These calculations have been made for $M = 1, r = 1.817\,6943, L = 5.645\,01$, corresponding to the values used in [4]. The law given by equation (17) concerns an infinite chain. It is interesting to numerically determine the number of bound states N_b for a *finite* linear chain with N centres in order to appreciate the rapidity of convergence when $N \to \infty$. The calculations have been made for a chain with ten and five centres only ($N = 10, 5$) with the previous parameter values of M, r, L, and for the λ values corresponding to $\rho = 0, 1/5, 2/5, 3/5, 4/5, 1$ in figure 1. For $N = 10$ and for the three cases, $\ell = m = 0$, $\ell = 1, |m| = 0, 1$, it has been found that $N_b = 0, 2, 4, 6, 8, 10$, for $\lambda(0), \lambda\left(\frac{1}{5}\right), \lambda\left(\frac{2}{5}\right), \lambda\left(\frac{3}{5}\right), \lambda\left(\frac{4}{5}\right), \lambda(1)$ respectively. For $N = 5$ and for the three cases, $\ell = m = 0$, $\ell = 1, |m| = 0, 1$, it has been found that $N_b = 0, 1, 2, 3, 4, 5$, for $\lambda(0), \lambda\left(\frac{1}{5}\right), \lambda\left(\frac{2}{5}\right), \lambda\left(\frac{3}{5}\right), \lambda\left(\frac{4}{5}\right), \lambda(1)$ respectively. The law given by equation (17) is therefore useful already for such low N values, for these parameter values.

If each interaction V_j centred at each point P_j is required to be invariant under all rotations of centre P_j, then each V_j must be of the form [3]

$$\lambda r^3 \exp(-\mathrm{i}j\mathbf{L}\cdot\mathbf{p}) \left\{ \sum_{m=-\ell}^{\ell} |r, \ell, m\rangle\langle r, \ell, m| \right\} \exp(\mathrm{i}j\mathbf{L}\cdot\mathbf{p}).$$

In that case, the spectrum is the union of the spectra corresponding to each different $|m|$ value, since ℓ_z commutes with H_ℓ^m. For fixed λ, r, L, ℓ values, the proportion $0 \leqslant \rho \leqslant 1$ of bound states is then obtained as follows: for each $|m|$ value between 0 and ℓ, one first determines λ_0 and λ_1 corresponding respectively to $\varrho = 0$, and $\varrho = 1$ in equation (17). Then, if $\lambda \geqslant \lambda_0$, one has $\varrho_m = 0$, and if $\lambda \leqslant \lambda_1$, one has $\varrho_m = 1$. Finally if $\lambda_1 < \lambda < \lambda_0$, one determines ϱ_m according to equation (17). The proportion of bound states is then expressed as

$$\begin{aligned}\rho &= \frac{1}{2\ell+1} \sum_{m=-\ell}^{\ell} \rho_m \\ &= \frac{1}{2\ell+1} \left[\rho_0 + 2 \sum_{m=1}^{\ell} \rho_m \right].\end{aligned}$$

Table 1. First line: β. Last line: $f(1, \beta)$, see equation (14). The three other lines: the first column gives the order N of the matrix $T_N(1)$, see equation (6); the second column gives the highest eigenvalues of $T_N(1)$; the other five columns give the eigenvalues of $T_N(1)$ numbered βN when all eigenvalues are sorted in decreasing order, with running number from 1 to N.

β	0	1/5	2/5	3/5	4/5	1
10	3.945 47	1.559 86	−0.024 7856	−0.776 527	−1.181 59	−1.364 25
100	8.514 12	1.017 35	−0.294 93	−0.944 823	−1.276 78	−1.386 05
1000	13.117 4	0.967 87	−0.320 663	−0.960 674	−1.285 03	−1.386 29
$f(1, \beta)$	∞	0.962 424	−0.323 507	−0.962 424	−1.285 93	−1.386 29

4.2.2. The case of s wave ($\ell = 0$). The case $\ell = 0$ is a particular case because the series $\sum_{j=1}^{\infty} \frac{\cos(j\pi\rho)}{j}$ diverges for $\rho = 0$. For $\rho \neq 0$, the sum of the series of equation (17) can be expressed in terms of a logarithm function [16]

$$2 \sum_{j=1}^{\infty} \frac{\cos(j\pi\rho)}{j} = -\ln[2(1 - \cos(\pi\rho))] \tag{18}$$

and therefore

$$\frac{1}{\lambda} = -2Mr^2 \{1 - \alpha \ln[2(1 - \cos(\pi\rho))]\} \qquad \text{if} \quad \ell = 0. \tag{19}$$

One deduces that ${}_{\infty}H_0^0$ always supports a bound state however close $\lambda < 0$ may be to zero, however large the intercentre distance L, and however small the range parameter r. Finally, if $\lambda \leqslant -\{2Mr^2[1 - \alpha \ln(4)]\}^{-1}$, then $\rho = 1$.

5. Mathematical results

By comparison of equations (7) and (13), one deduces that the spectrum $S(2\ell + 1)$ ($\ell = 0, 1, 2, \ldots$) of the Toeplitz matrix $T(2\ell + 1)$ (6) is given by

$$S(2\ell + 1) = \{f(2\ell + 1, \beta) \mid 0 \leqslant \beta \leqslant 1\}. \tag{20}$$

The density of states (eigenvectors) corresponds to a uniform density for the variable β in the interval $0 \leqslant \beta \leqslant 1$. This corresponds to the fact that different points in the reduced Brillouin zone have the same weight, or, otherwise stated, there is no privileged unitary irreducible representation of the translation group. From $\left|\frac{\cos(j\pi\beta)}{j^{2\ell+1}}\right| \leqslant \frac{1}{j^{2\ell+1}}$, and from the convergence of the series $\sum_{j=1}^{\infty} j^{-(2\ell+1)}$ if $\ell \neq 0$, it follows that the series (14) is normally convergent if $\ell \neq 0$. As normal convergence implies uniform convergence, the integral

$$2 \int_0^1 \left\{ \sum_{j=1}^{\infty} \frac{\cos(j\pi\beta)}{j^{2\ell+1}} \right\} \mathrm{d}\beta$$

can be made term-by-term and thus clearly yields 0. Taking into account a uniform density in β, this integral evaluates the trace, and the expected zero-trace property for a bound spectrum is thus manifested.

In order to appreciate the behaviour of the convergence, as N increases, of the spectra of the matrix $T_N(2\ell + 1)$ of order N (see equation (6)) towards the expected spectra given by equation (20), tables 1, 2 report some numerically computed eigenvalues compared to numerical values of $f(2\ell + 1, \beta)$ for $\ell = 0$ (table 1) and for $\ell = 1$ (table 2). (In table 1, $f(1, \beta)$ is given by equation (18).)

Table 2. As in table 1, but for $\ell = 1$, so that $f(2\ell+1, \beta)$ and $T_N(2\ell+1)$ now read $f(3, \beta)$ and $T_N(3)$.

β	0	1/5	2/5	3/5	4/5	1
10	2.213 86	1.780 27	0.657 144	−0.448 403	−1.293 11	−1.745 23
100	2.399 84	1.644 41	0.408 572	−0.729 691	−1.510 361	−1.802 41
1000	2.404 05	1.629 11	0.381 74	−0.758 684	−1.530 5	−1.803 08
$f(3, \beta)$	2.404 11	1.627 39	0.378 736	−0.761 913	−1.532 71	−1.803 09

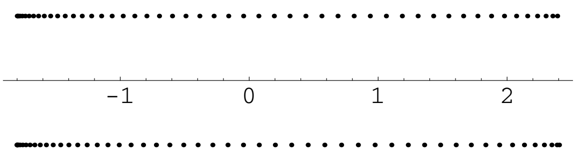


Figure 2. Above the horizontal axis: eigenvalues of $T_{50}(3)$ (see equation (6)), to be compared, below the horizontal axis, with $2\sum_{j=1}^{\infty}\cos(j\pi\frac{k}{49})/j^3$ for $k = 0, 1, 2, \ldots, 49$.

In order to appreciate visually that the density of states in equation (20) corresponds to a uniform density in β, all the numerically computed eigenvalues of $T_{50}(3)$ (see equation (6)) are reported in figure 2, above the horizontal axis, together with, below the horizontal axis, $2\sum_{j=1}^{\infty}\cos\left(j\pi\frac{k}{49}\right)\big/j^3$ for $k = 0, 1, 2, \ldots, 49$, i.e. a uniform distribution with respect to β. It is clear that the distribution of the numerically computed eigenvalues agrees with an uniform distribution with respect to β of $2\sum_{j=1}^{\infty}\cos(j\pi\beta)/j^3$.

Except for the case $\ell = 0$, the spectrum is bound. This was expected since all the Geršgorin discs [14] of the matrices $T_N(2\ell+1)$ are centred on the origin and their maximum radius converges to $2\zeta(2\ell+1)$ when $N \to \infty$ for $\ell \neq 0$, and diverges for $\ell = 0$. Taking into account a uniform density in β, the zero-trace property can nevertheless be explicitly verified for $\ell = 0$ from equation (18) since

$$-\int_0^1 \ln[2(1-\cos(\pi\beta))]\,\mathrm{d}\beta = 0.$$

6. Mathematical digression

In this section we examine, mostly by numerical diagonalization, how the spectra of large *truncated* Toeplitz matrices $T(s)$ given by equation (4), are related to

$$S(s) = \{f(s, \beta) \mid 0 \leqslant \beta \leqslant 1\} \tag{21}$$

for values of s different from $2\ell+1$, including complex values.

To avoid repetitions, we note from now on that the series $2\sum_{j=1}^{\infty}\cos(j\pi\beta)/j^s$ converges uniformly for $\mathrm{Re}(s) > 1$, and that the zero-trace property is then verified by term-by-term integration: $\int_0^1\cos(j\pi\beta)\,\mathrm{d}\beta = 0$. For $\mathrm{Re}(s) \leqslant 1$, $\beta = 0$ is a singularity.

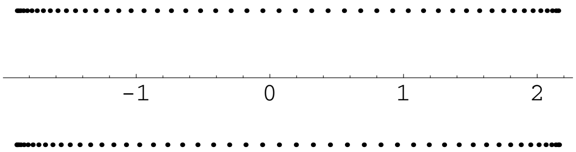


Figure 3. Above the horizontal axis: eigenvalues of $T_{50}(4)$ (see equation (6)), to be compared, below the horizontal axis, with $2\sum_{j=1}^{\infty}\cos(j\pi\frac{k}{49})/j^4$ for $k = 0, 1, 2, \ldots, 49$.

6.1. *Zero or even positive values of s*

For $s = 2k$, $k = 0, 1, \ldots, \infty$, the spectrum given by equation (21) can be expressed in terms of Bernoulli polynomials B_n defined by

$$\frac{t\exp(xt)}{\exp(t)-1} = \sum_{k=0}^{\infty} B_k(x)\frac{t^k}{k!}.$$

One obtains (see equation (9.622) of [16], or [20])

$$S(2k) = \left\{(-1)^{k-1}\,\frac{(2\pi)^{2k}}{(2k)!}B_{2k}\left(\frac{\beta}{2}\right)\middle|\,0 \leqslant \beta \leqslant 1\right\}. \tag{22}$$

6.1.1. Zero value of s. For $k = 0$ (i.e. the non-integer value $\ell = -\frac{1}{2}$ in equation (20)), equation (22) gives

$$S(0) = \{-1\}. \tag{23}$$

Now, it is easy to determine the spectrum of the corresponding truncated Toeplitz matrix $T_N(0)$ since this matrix has zero on the main diagonal and unity elsewhere. If this matrix corresponds to a linear operator $\mathcal{T}$ with respect to the basis e_i, $i = 1, \ldots, N$, then one can easily verify that the $N-1$ vectors $e_1 - e_i$, $i = 2, \ldots, N$ are eigenvectors of $\mathcal{T}$ with eigenvalue -1. The remaining vector $\sum_{i=1}^{N} e_i$ of the new basis is an eigenvector with eigenvalue $N-1$. Thus the spectrum is $\{-1, N-1\}$ in the finite case. If we consider the limit $N \to \infty$, it is clear that $\lim_{N\to\infty}\sum_{i=1}^{N} e_i$ does not converge, and that there is no eigenvector corresponding to non-zero eigenvalue. The spectrum in the infinite limit can thus be appropriately considered to be the zero point only, as given by equation (23). The zero-trace property of finite matrices is therefore not manifested as the sum of eigenvalues in the limit $N \to \infty$.

It is seen that the general result given by equation (21) may discard infinite points, a fact that will be recurrent from now on when some of the eigenvalues of the truncated Toeplitz matrix $T_N(s)$ diverge as $N \to \infty$. As a consequence, the zero-trace property of finite matrices may not always correspond to zero values of the integrals $\int_0^1 f(s,\beta)\,\mathrm{d}\beta$.

6.1.2. Strictly positive even values of s. Numerical diagonalizations of truncated Toeplitz matrices have confirmed equation (22) for some k values. Figure 3 provides an illustration for $s = 2k = 4$, and $N = 50$.

6.2. *Negative integer values of s*

For $s = -n$, a negative integer, one has [15]

$$Li_{-n}(z) = \left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^n \frac{z}{1-z}$$

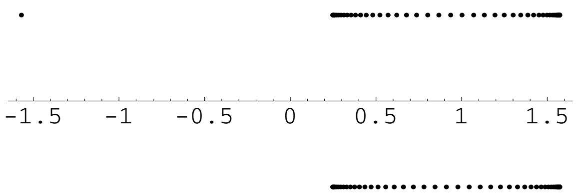


Figure 4. Above the horizontal axis: arctangent of the eigenvalues of $T_{50}(-3)$ (see equation (6)), to be compared, below the horizontal axis, with the arctangent of the right-hand side of equation (28) where $\beta = \frac{k}{49}$ for $k = 0, 1, 2, \ldots, 49$.

and therefore

$$Li_{-n}(\exp(\mathrm{i}\pi\beta)) = \frac{(-\mathrm{i})^{n-1}}{2\pi^n}\left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n [\cot(\pi\beta/2)] \tag{24}$$

$$f(-n, \beta) = \frac{(-\mathrm{i})^{n-1}}{2\pi^n}\left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^n \{\cot(\pi\beta/2)[1 - (-1)^n]\} \tag{25}$$

which is clearly zero if n is even.

6.2.1. Negative even integer values. For negative even integer values of s, $s = -2k$, $k = 1, 2, \ldots, \infty$, equation (25) thus gives

$$S(-2k) = \{0\}. \tag{26}$$

It has been verified for some k, N values that the corresponding truncated Toeplitz matrix of order N has a kernel of dimension equal to $N - 2k - 1$. The absolute values of the $2k$ non-zero eigenvalues increase rapidly with N, and therefore result (26) is expected. We shall not study further this particular interesting case in the present paper.

6.2.2. Negative odd integer values. For negative odd integer values of s, $s = -2k - 1$, $k = 0, 1, \ldots, \infty$, equation (24) gives

$$S(-2k-1) = \left\{ \frac{(-1)^k}{\pi^{2k+1}}\left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^{2k+1} \cot(\pi\beta/2) \,\middle|\, 0 \leqslant \beta \leqslant 1 \right\}. \tag{27}$$

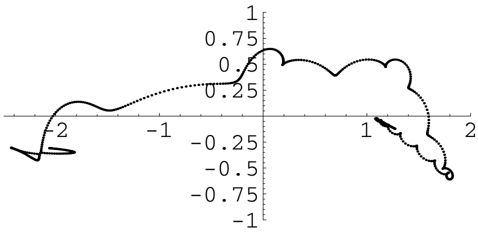
Numerical diagonalizations of truncated Toeplitz matrices have confirmed equation (27) for some k values. As the spectrum is unbounded, we apply the function arctangent to rescale the real line between $\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. Figure 4 provides an illustration for $s = -2k - 1 = -3$, and $N = 50$,

$$\frac{(-1)}{\pi^3}\left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^3 \cot(\pi\beta/2) = \frac{2 + \cos(\pi\beta)}{4\left[\sin\left(\frac{\pi\beta}{2}\right)\right]^4}. \tag{28}$$

Two eigenvalues of the truncated T_{50} matrix whose arctangent is close to $-\frac{\pi}{2}$ ensure the zero-trace property of the truncated T_{50} matrix, and have no images in the infinite limit.

6.3. Arbitrary complex values of s

The numerically computed eigenvalues of the truncated Toeplitz matrix of order 500, $T_{500}(1.5 + \mathrm{i}49)$ are reported at the top of figure 5, whereas the lower graph of this figure reported $2\sum_{j=1}^{\infty} \cos\left(j\pi\frac{k}{499}\right)/j^{1.5+\mathrm{i}49}$, $k = 0, 1, 2, \ldots, 499$. It is clear that the general



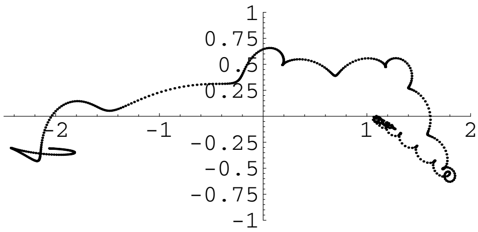


Figure 5. Top graph: eigenvalues of $T_{500}\,(1.5 + \mathrm{i}49)$, see equation (6), in the complex plane. Bottom graph: $f(1.5 + \mathrm{i}49, \frac{k}{499})$ for $k = 0, 1, \ldots, 499$, see equation (14), in the complex plane.

behaviour, including the density of states, is obtained. The small disagreements which are visible near the right extremity of the spectrum indicate that the convergence is slower in this region.

6.4. Spectral interpretation of the zeros of the Riemann zeta function

From now on, we consider that s belongs to the critical strip $0 < \mathrm{Re}(s) < 1$. In that case, $f(s, 0)$ cannot be considered to be the limit of $f(s, \beta)$ when $\beta \to 0$ because $\beta = 0$ is a singularity. Let us go over to the spectrum $S(s)$ of $T(s)$ starting from $\beta = 1$. When s is a zero of the Riemann zeta function, equation (16e) tells us that we start at the origin of the complex plane. As β decreases, we describe in the complex plane a curve which crosses the origin three times, when $\beta = \frac{2}{3}, \frac{1}{2}, \frac{1}{3}$, according to equations (16d), (16c), (16b). The zeros of the Riemann zeta function are thus interpreted as multiple points of the spectrum of the Toeplitz matrix $T(s)$. Figure 6 shows the spectrum for the first non-trivial zero of the Riemann zeta function, $s \simeq 1/2 + \mathrm{i}14.134\,725$. Let us first consider the bottom graph corresponding to $f(1/2 + \mathrm{i}14.134\,725, \beta)$. As β starts to decrease from unity, one leaves the origin slightly below the negative real axis, and then moves clock-wise. One crosses the origin three times again, and, as β approaches zero, the curves spiral with increasing radius, and therefore the values for k smaller than about 30 are not visible in this curve. The top graph, corresponding to the numerically computed eigenvalues of $T_{500}(1/2 + \mathrm{i}14.134\,725)$, exhibits the same general behaviour, including density of states. One sees that the convergence to $f(1/2 + \mathrm{i}14.134\,725, \beta)$ becomes slower as β decreases.

7. Summary and conclusions

For the Hamiltonian ${}_N H = \frac{p^2}{2M} + \lambda \sum_{j=1}^{N} |\xi_j\rangle\langle\xi_j|$, it has been shown that at most N (the number of projectors) bound states exist. For an infinite linear chain, this Hamiltonian takes the form given by equations (1), (2), (3). For fixed values of ℓ, m, there are then three parameters in this Hamiltonian: the interaction range parameter r, the intercentre distance parameter L

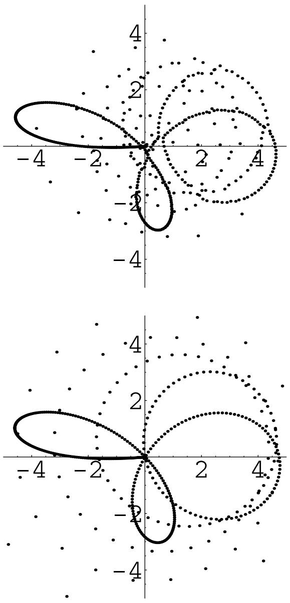


Figure 6. Top graph: eigenvalues of T_{500} $(1/2 + \mathrm{i}14.134\,725)$, see equation (6)), in the complex plane. Bottom graph: $f\left(1/2 + \mathrm{i}14.134\,725, \frac{k}{499}\right)$ for $k = 0, 1, \ldots, 499$, see equation (14), in the complex plane. The values corresponding to k smaller than about 30 are not visible since the corresponding points spiral with increasing radii and are outside the figure.

(with $0 < r/L \leqslant 1/2$) and the strength interaction parameter λ. The following question has been addressed: for given values of r, L, what is the value of the remaining parameter λ if one requires that the limit when $N \to \infty$ of the ratio of the number of bound states to the total number of centres, N_b/N, takes an arbitrary fixed value ρ $(0 \leqslant \rho \leqslant 1)$? The answer is given by equation (17) with $\alpha = r/L$, the function g_ℓ^m defined by equation (8) and the function f defined by equation (14). To solve this question, we have been led to consider the spectra of doubly infinite Toeplitz matrices given by equation (4) with $s = 2\ell + 1 = 1, 3, 5, \ldots.$ The spectra are given by

$$S\,(2\ell + 1) = \left\{ 2 \sum_{n=1}^{\infty} \frac{\cos\,(n\pi\beta)}{n^{2\ell+1}} \,\middle|\, 0 \leqslant \beta \leqslant 1 \right\}.$$

The density of states corresponds to a uniform density for β. From a physicist point of view this follows from the interpretation of β as position coordinate in the reduced Brillouin zone. In section 6, we examine how numerical diagonalization of *truncated* Toeplitz matrices (4) converges to the expression $S(s)$ for some s values different from $2\ell + 1$. In particular, this leads to interpret the zeros of the Riemann function $\zeta(s)$ in the critical strip $0 < \mathrm{Re}(s) < 1$ as multiple points (at the origin) of the spectra of the Toeplitz matrices given by equation (4).

Let us conclude with the types of physical problems related to this work. The model used in this paper is that proposed in [3]. This model is exactly solvable for an arbitrary geometrical configuration of a *finite* number of centres. This sentence means that energy eigenvalues are the zeros of a determinant of a matrix of order N (the number of projectors) whose matrix elements are simple analytical functions. The search for the zeros however required numerical calculations. Once the energy eigenvalues are determined, the eigenfunctions can be determined exactly. In the present paper, we derive an exact result (equation (17)) concerning the proportion of bound states for one *infinite* system: a periodic linear chain. It has been verified that this result may be useful for estimating *a priori* (i.e. without performing the search for zeros which gives the energy of the bound states) the number of bound states of a finite linear chain, even with a small number of centres. It would be interesting to extend the present work to other infinite systems, in particular Fibonacci chains and Penrose structures. One then expects that the strength interaction parameter λ as function of the proportion of bound states ρ will exhibit gap structures analogous to the energy gap structures. It may be easier to quantify λ subject to the boundary condition of the occurrence of a zero-energy bound state, than to quantify the energy directly.

Appendix A. Evaluation of a series

This appendix only gives the principal steps which allow us to go from equations (11) to (A.4) for $0 < \alpha \leqslant \frac{1}{2}$ and $0 < \beta \leqslant 1$, without giving all detailed justifications of the steps. The previous inequalities ensure that $|2n + \beta|\,\pi\alpha > 0$. In order to avoid the display of too many formulae, we sometimes refer directly to the equation numbers pertaining to the references cited.

To evaluate the series of integrals defined by equation (11) we start from an integral representation of the square of a regular spherical Bessel function [16, 17]:

$$j_\ell^2(x) = \frac{1}{2x}\int_0^\pi \sin\left[2x\sin\left(\frac{\varphi}{2}\right)\right] P_\ell\left[\cos(\varphi)\right]\cos\left(\frac{\varphi}{2}\right)\mathrm{d}\varphi. \tag{A.1}$$

As $P_\ell^m(-z) = (-1)^{\ell+m} P_\ell^m(z)$ [8], the square $\left[P_\ell^m(z)\right]^2$ is an even function of z, and $(2n+\beta)$ can be replaced by $|2n+\beta|$ in the argument of equation (11),

$$A_\ell^m(\alpha,\beta) = \sum_{n=-\infty}^{\infty}\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{\mathrm{d}x}{x}\left|P_\ell^m\left(\frac{|2n+\beta|\,\pi\alpha}{x}\right)\right|^2$$
$$\times\frac{1}{2x}\int_0^\pi \sin\left[2x\sin\left(\frac{\varphi}{2}\right)\right] P_\ell\left[\cos(\varphi)\right]\cos\left(\frac{\varphi}{2}\right)\mathrm{d}\varphi.$$

For each n, the integrand, to be denoted by $g(x,\varphi)$, is a continuous function on the region $D = [|(2n+\beta)|\,\pi\alpha, \infty[\times[0,\pi]$. The argument of P_ℓ^m varies between 1 and 0, and then it is easy to show that $|g(x,\varphi)| < K/x^2$, with K a constant. The integral of K/x^2 over the domain D converges, and therefore the integral $\int_{|(2n+\beta)|\pi\alpha}^{\infty} g(x,\varphi)\,\mathrm{d}x$ is normally convergent for $\varphi \in [0,\pi]$. Normal convergence implies uniform convergence, and the latter allows us to interchange the order of integration which will be made below.

Before interchanging the order of integration, consider the effect of splitting the interval of integration $[0,\pi]$ over φ into two intervals, $[0,\varepsilon]$ and $[\varepsilon,\pi]$, and let us verify explicitly that the contribution, to be denoted by $C(\varepsilon)$ to $A_\ell^m(\alpha,\beta)$ of the interval $[0,\varepsilon]$ goes to zero as $\varepsilon \to 0^+$. To first order in ε: $P_\ell[\cos(\varphi)] = 1 + O(\varphi^2)$, and the integral becomes

$$\int_0^\varepsilon \sin\left[2x\sin(\varphi/2)\right]\cos(\varphi/2)\,\mathrm{d}\varphi = \frac{2\sin^2\left[x\sin\left(\frac{\varepsilon}{2}\right)\right]}{x}.$$

Let K be a majorant of $\left|P_\ell^m(z)\right|^2$ when $0 \leqslant z \leqslant 1$. Then

$$|C(\varepsilon)| \leqslant K\sum_{n=-\infty}^{\infty}\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{\mathrm{d}x}{x^3}\sin^2\left[x\sin\left(\frac{\varepsilon}{2}\right)\right]$$
$$\leqslant K\sum_{n=-\infty}^{\infty}\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{\mathrm{d}x}{x^3} \leqslant K'$$

with K' a finite number independent of ε. It follows that $C(\varepsilon)$ can be majorized to any prescribe accuracy by the finite sum $K\sum_{n=-N}^{N}\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{dx}{x^3}\sin^2\left[x\sin\left(\frac{\varepsilon}{2}\right)\right]$ and this finite sum tends to zero when $\varepsilon\to 0^+$ since each of its terms goes to zero. Thus one has

$$A_\ell^m(\alpha,\beta)=\lim_{\varepsilon\to 0^+}\sum_{n=-\infty}^{\infty}\int_\varepsilon^\pi d\varphi\int_{|(2n+\beta)|\pi\alpha}^{\infty}\frac{dx}{x}\left|P_\ell^m\left(\frac{|2n+\beta|\,\pi\alpha}{x}\right)\right|^2 \times\frac{1}{2x}\sin\left[2x\sin\left(\frac{\varphi}{2}\right)\right]P_\ell\left[\cos(\varphi)\right]\cos\left(\frac{\varphi}{2}\right).$$

The square of the associated Legendre polynomial $P_\ell^m(z)$ is a polynomial in the variable z^2 of degree ℓ [8]:

$$\left|P_\ell^m(z)\right|^2=\sum_{k=0}^{\ell}p_k^m z^{2k}.$$

The change of variable $X=2x\sin\left(\frac{\varphi}{2}\right)$ then yields

$$A_\ell^m(\alpha,\beta)=\lim_{\varepsilon\to 0^+}\sum_{n=-\infty}^{\infty}\frac{1}{2}\sum_{k=0}^{\ell}p_k^m\int_\varepsilon^\pi d\varphi P_\ell\left[\cos(\varphi)\right]\cos\left(\frac{\varphi}{2}\right)\left[2\sin\left(\frac{\varphi}{2}\right)\right]^{2k+1} \times\left\{\left[|2n+\beta|\,\pi\alpha\right]^{2k}\int_{|(2n+\beta)|2\pi\alpha\sin\left(\frac{\varphi}{2}\right)}^{\infty}dX\frac{\sin(X)}{X^{2(k+1)}}\right\}.$$

The change of variable $v=\frac{X}{|2n+\beta|}$ for the term inside the curly braces leads to the expression

$$(\pi\alpha)^{2k}\left\{\frac{1}{|2n+\beta|}\int_{2\pi\alpha\sin\left(\frac{\varphi}{2}\right)}^{\infty}dv\frac{\sin(|2n+\beta|\,v)}{v^{2(k+1)}}\right\}.$$

Integration by parts of this last expression yields

$$\frac{(\pi\alpha)^{2k}}{2k+1}\left\{\frac{1}{\left[2\pi\alpha\sin\left(\frac{\varphi}{2}\right)\right]^{2k+1}}\left[\frac{\sin\left[2\pi\alpha\sin\left(\frac{\varphi}{2}\right)|2n+\beta|\right]}{|2n+\beta|}\right] +\left[\int_{2\pi\alpha\sin\left(\frac{\varphi}{2}\right)}^{\infty}dv\frac{\cos(v\,|2n+\beta|)}{v^{2k+1}}\right]\right\}$$

so that

$$A_\ell^m(\alpha,\beta)=\lim_{\varepsilon\to 0^+}\sum_{n=-\infty}^{\infty}\frac{1}{2}\sum_{k=0}^{\ell}\frac{p_k^m}{2k+1}\int_\varepsilon^\pi d\varphi P_\ell\left[\cos(\varphi)\right]\cos\left(\frac{\varphi}{2}\right) \times\left\{\frac{1}{(\pi\alpha)}\left[\frac{\sin\left[2\pi\alpha\sin\left(\frac{\varphi}{2}\right)|2n+\beta|\right]}{|2n+\beta|}\right] +(\pi\alpha)^{2k}\left[2\sin\left(\frac{\varphi}{2}\right)\right]^{2k+1}\left[\int_{2\pi\alpha\sin\left(\frac{\varphi}{2}\right)}^{\infty}dv\frac{\cos(v\,|2n+\beta|)}{v^{2k+1}}\right]\right\}.$$

The first term inside the curly braces is k independent. After term-by-term integration of $\int_{-1}^{1}\left[P_\ell^m(x)\right]^2 dx$, the orthonormality relations for associated Legendre polynomials yield

$$\sum_{k=0}^{\ell}\frac{p_k^m}{2k+1}=\frac{(\ell+m)!}{(2\ell+1)(\ell-m)!}$$

$$A_\ell^m(\alpha,\beta) = \lim_{\varepsilon\to 0^+} \sum_{n=-\infty}^{\infty} \frac{1}{2}\int_\varepsilon^\pi \mathrm{d}\varphi P_\ell[\cos(\varphi)]\cos\left(\frac{\varphi}{2}\right)$$
$$\times \left\{ \frac{(\ell+m)!}{(2\ell+1)(\ell-m)!}\frac{1}{(\pi\alpha)}\left[\frac{\sin\left[2\pi\alpha\sin\left(\frac{\varphi}{2}\right)|2n+\beta|\right]}{|2n+\beta|}\right]\right.$$
$$\left. + \sum_{k=0}^{\ell}\frac{p_k^m}{2k+1}(\pi\alpha)^{2k}\left[2\sin\left(\frac{\varphi}{2}\right)\right]^{2k+1}\left[\int_{2\pi\alpha\sin\left(\frac{\varphi}{2}\right)}^{\infty}\mathrm{d}v\frac{\cos(v|2n+\beta|)}{v^{2k+1}}\right]\right\}. \tag{A.2}$$

The interchange of the order of integration and of summation in the first term inside the curly braces of equation (A.2) leads to the evaluation of a trigonometric series

$$\sum_{n=-\infty}^{\infty}\frac{\sin[(2n+\beta)\gamma]}{2n+\beta} = \frac{\pi}{2} \qquad \text{for} \quad 0<\gamma = 2\pi\alpha\sin\left(\frac{\varphi}{2}\right) < \pi. \tag{A.3}$$

From $\left|\sum_{n=j}^{m}\exp(\mathrm{i}nx)\right| \leqslant 2/|\exp(\mathrm{i}x)-1|$ for $x\neq 2k\pi$, and for $k, j, m \in \mathbb{Z}$, and from the decrease to zero of the sequence $1/|2n+\beta|$ as $n\to\infty$, one can use the Abel criterion (see e.g. [18]) to show the uniform convergence of this series on every closed interval which does not contain $2k\pi$. This justifies the interchange of the order of integration and summation. Result (A.3) follows after some elementary calculations from (see e.g. equation 12.5.1 of [19])

$$\sum_{n=-\infty}^{\infty}\frac{\exp(\mathrm{i}n\theta)}{n-a} = -2\pi\mathrm{i}\frac{\exp(\mathrm{i}a\theta)}{\exp(\mathrm{i}a2\pi)-1} \qquad \text{if} \quad 0<\theta<2\pi.$$

The interchange of the order of integration and of summation in the second term inside the curly braces of equation (A.2) leads to the evaluation of a trigonometric series which produces a series of Dirac distributions:

$$\sum_{n=-\infty}^{\infty}\cos(v|2n+\beta|) = \pi\sum_{j=-\infty}^{\infty}\delta(v-j\pi)\cos(j\pi\beta).$$

This leads to

$$A_\ell^m(\alpha,\beta) = \frac{1}{2}\int_0^\pi \mathrm{d}\varphi P_\ell[\cos(\varphi)]\cos\left(\frac{\varphi}{2}\right)\left\{\frac{(\ell+m)!}{(2\ell+1)(\ell-m)!}\frac{1}{2\alpha}\right.$$
$$\left. + \sum_{k=0}^{\ell}\frac{p_k^m}{2k+1}(\pi\alpha)^{2k}\left[2\sin\left(\frac{\varphi}{2}\right)\right]^{2k+1}\pi\sum_{j=1}^{\infty}\left[\frac{\cos(j\pi\beta)}{(j\pi)^{2k+1}}\right]\right\}.$$

Now from equation (7.233) of [16]

$$\frac{1}{4\alpha}\int_0^\pi \mathrm{d}\varphi P_\ell[\cos(\varphi)]\cos\left(\frac{\varphi}{2}\right) = \frac{1}{(2\alpha)(2\ell+1)}.$$

The change of variable $x=\cos(\varphi)$ yields

$$\int_0^\pi \mathrm{d}\varphi P_\ell(\cos(\varphi))\cos\left(\frac{\varphi}{2}\right)\left(2\sin\left(\frac{\varphi}{2}\right)\right)^{2k+1} = 2^k\int_{-1}^{1}\mathrm{d}x P_\ell(x)(1-x)^k.$$

This last integral is zero if $k<\ell$ (see equation (7222.1) of [16]). For $k=\ell$, the change of variable $x\to -x$ yields from equation (7222.2) of [16]:

$$\int_0^\pi \mathrm{d}\varphi P_\ell(\cos(\varphi))\cos\left(\frac{\varphi}{2}\right)\left(2\sin\left(\frac{\varphi}{2}\right)\right)^{2\ell+1} = (-1)^\ell 2^{2\ell+1}\frac{(\ell!)^2}{(2\ell+1)!}.$$

$A_\ell^m(\alpha,\beta)$ can then be expressed as

$$A_\ell^m(\alpha,\beta) = \left\{ \frac{(\ell+m)!}{(2\ell+1)(\ell-m)!} \frac{1}{(2\alpha)(2\ell+1)} + \frac{p_\ell^m}{2\ell+1} (\alpha)^{2\ell} (-1)^\ell \, 2^{2\ell} \frac{(\ell!)^2}{(2\ell+1)!} \sum_{j=1}^{\infty} \left[\frac{\cos(j\pi\beta)}{j^{2\ell+1}} \right] \right\}.$$

Finally, from equation (2.5.17) of [8]

$$p_\ell^m = (-1)^m \left[\frac{(2\ell)!}{2^\ell \ell! \, (\ell-m)!} \right]^2$$

one obtains

$$A_\ell^m(\alpha,\beta) = \frac{1}{(2\ell+1)^2} \left\{ \frac{(\ell+m)!}{(\ell-m)!} \frac{1}{(2\alpha)} + (-1)^{\ell+m} \alpha^{2\ell} \frac{(2\ell)!}{[(\ell-m)!]^2} \sum_{j=1}^{\infty} \frac{\cos(j\pi\beta)}{j^{2\ell+1}} \right\}. \tag{A.4}$$

It is remarkable that the α dependence of $A_\ell^m(\alpha,\beta)$ splits into the sum of two power laws, and that the β dependence reduces to the series $2\sum_{j=1}^{\infty}\cos(j\pi\beta)\, j^{-(2\ell+1)}$. This series can be expressed in terms of the polylogarithm function Li_s defined by the series

$$Li_s(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^s} \tag{A.5}$$

when it converges, and by analytic continuation otherwise [20]. One has

$$2\sum_{j=1}^{\infty} \cos(j\pi\beta)\, j^{-(2\ell+1)} = Li_{2\ell+1}(\exp(\mathrm{i}\pi\beta)) + Li_{2\ell+1}(\exp(-\mathrm{i}\pi\beta)) \tag{A.6}$$

$$= f(2\ell+1,\beta). \tag{A.7}$$

The polylogarithm functions are also a particular case of the Lerch phi function $\Phi(z,s,a) = \sum_{j=0}^{\infty} \frac{z^j}{(a+j)^s}$ where any term with $a+j=0$ is excluded, by the relation $Li_s(z) = \Phi(z,s,0)$. For references on the polylogarithm functions, see e.g. [15, 20, 21].

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