Gaussian integration formulas for logarithmic weights and application to 2-dimensional solid-state lattices.

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Nothing exists per se *except atoms and the void*
... however solid objects seem,

Lucretius, *On the Nature of Things*,
Translated by William Ellery Leonard

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Abstract: The making of Gaussian numerical integration formulas is considered for weight functions with logarithmic singularities. Chebyshev modified moments are found most convenient here. The asymptotic behaviour of the relevant recurrence coefficients is stated in a conjecture. The relation with the recursion method in solid-state physics is summarized, and more details are given for some two-dimensional lattices (square lattice and hexagonal (graphene) lattice).

Contents

1. Orthogonal polynomials and Gaussian quadrature formulas.

Let μ be a positive measure on a real interval $[a, b]$, and P_n the related monic orthogonal polynomial of degree n, i.e., such that

$$P_n(x) = x^n + \cdots \ , \ \int_a^b P_n(t)P_m(t)d\mu(t) = 0, m \neq n, \quad n = 0, 1, \dots \tag{1}$$

An enormous amount of work has been spent since about 200 years on the theory and the applications of these functions. One of their most remarkable properties is the recurrence relation

$$P_{n+1}(x) = (x - b_n)P_n(x) - a_n^2 P_{n-1}(x), \quad n = 1, 2, \dots, \tag{2}$$

with $P_1(x) = x - b_0$. See, among numerous other sources, Chihara's book [13], Gautschi's one [27], chap. 18 of NIST handbook [60].

Orthogonal polynomials are critically involved in the important class of Gaussian integration formulas. A classical integration formula (Newton-Cotes, Simpson, etc.) $\int_a^b f(t)d\mu(t) \approx w_1 f(x_1) + \cdots + w_N f(x_N)$ is the integral $\int_a^b p(t)\ d\mu(t)$ of the polynomial interpolant p of f at the points $x_1, \dots, x_N$. Interpolation errors can sometimes become quite wild, to the opposite of least squares approximations made with a polynomial q minimizing $\int_a^b (f(t) - q(t))^2 d\mu(t) \Rightarrow \int_a^b (f(t) - q(t))r(t)\, d\mu(t) = 0$ for any polynomial r of degree $< N$. We want the favorable aspects of both sides! i.e., easy use of numerical integration formulas, and safety of least squares approximation. Take at least for f a polynomial of degree N, see that $f - p$ vanishes at $x_1, \dots, x_N$ and will be orthogonal to all polynomials of degree $< N$ if it is a constant times P_N, so if $x_1, \dots, x_N$ are the zeros of P_N. All least squares problems are then satisfactorily solved with the discrete scalar product $(f, g)_N = \sum_1^N w_j f(x_j)g(x_j)$. See Davis & Rabinowitz [17, § 2.7], Boyd [7, chap. 4] for this discussion.

Approximate integration formulas are not only used in area or volume calculations from time to time, they are also used massively in pseudospectral solutions of big partial derivative equations and other functional equations. As an example of numerical procedure, a polynomial approximation to the solution of a functional equation $F(u) = 0$ is determined by orthogonality conditions $\int_a^b F(u(t))r(t)\, d\mu(t) = 0$ for any polynomial r of degree $< N$ (Galerkin method), where the integral is replaced by its Gaussian formula $(F(u), r)_N = 0$. See for instance Boyd [7, chap. 3, 4], Fornberg [21, § 4.7], Mansell & al. [51], Shizgal [66].

2. Power moments and recurrence coefficients.

2.1. Recurrence coefficients and examples.

Let us consider the generating function of the moments μ_n, which is called here the Stieltjes function of the measure $d\mu$

$$S(x) = \int_a^b \frac{d\mu(t)}{x-t} = \frac{\mu_0}{x} + \frac{\mu_1}{x^2} + \cdots, x \notin [a,b], \quad \mu_n = \int_a^b t^n d\mu(t). \tag{3}$$

Sometimes, S is called the Stieltjes transform of $d\mu$, but technically, the Stieltjes transform of a measure is the integral of $(x+t)^{-1}d\mu(t)$ on the positive real line [38, chap. 12]. For measures on the whole real line, one should use the name "Hamburger transform". P. Henrici [39, §14.6] speaks of "Cauchy integrals on straight line segments", Van Assche [69] calls S "Stieltjes transform" for (3) in all cases.

The power expansion (3) is an asymptotic expansion. If $[a,b]$ is finite, the expansions converges when $|x| > \max(|a|,|b|)$.

The function S is also the first function of the second kind $Q_n(x) = \displaystyle\int_a^b \frac{P_n(t)\,d\mu(t)}{x-t}$. The recurrence relation (2) holds for the Q_ns too. Indeed, $Q_{n+1}(x) = \displaystyle\int_a^b \frac{[(t-b_n = t-x+x-b_n)P_n(t) - a_n^2 P_{n-1}(t)]\,d\mu(t)}{x-t} = -\mu_0\delta_{n,0} + (x-b_n)Q_n(x) - a_n^2 Q_{n-1}(x)$. At $n=0$, $Q_1(x) - (x-b_0)Q_0(x) + \mu_0 = 0$. We have $\dfrac{Q_n(x)}{Q_{n-1}(x)} = \dfrac{a_n^2}{x-b_n-\dfrac{Q_{n+1}(x)}{Q_n(x)}}$, [29, eq. (2.15)]and $S(x) = Q_0(x) = \dfrac{\mu_0}{x-b_0-\dfrac{a_1^2}{x-b_1-\ddots\dfrac{Q_{n+1}(x)}{Q_n(x)}}}$. For bounded $[a,b]$, the continued fraction converges for all $x \notin [a,b]$ [39,72].

Some examples, which will be inspiring later on, are

$$S(x) = \frac{1}{2}\int_{-1}^1 \frac{dt}{x-t} = \frac{1}{2}\log\frac{x+1}{x-1} = \frac{1}{x} + \frac{1}{3x^3} + \frac{1}{5x^5} + \cdots \tag{4}$$

$$S(x) = \int_{-1}^1 \frac{|t|dt}{x-t} = \int_0^1 \frac{2txdt}{x^2-t^2} = x\log\frac{x^2}{x^2-1} = \frac{1}{x} + \frac{1}{2x^3} + \frac{1}{3x^5} + \cdots \tag{5}$$

This shows how logarithmic singularities are often seen in Stieltjes functions.

Here is a case with an explicit logarithmic singularity in the weight function

$$S(x) = -\int_0^1 \frac{\log t\,dt}{x-t} = \mathrm{Li}_2(x^{-1}) = \sum_1^\infty \frac{1}{n^2\,x^n}, \tag{6}$$

where Li_2 is the dilogarithm function [60, §25.12].

A last example with Euler's Beta function:

$$S(x) = \int_0^1 \frac{t^{q-1}(1-t)^{p-q}\,dt}{x-t} = \frac{\mu_0}{x} + \frac{\mu_1}{x^2} + \frac{\mu_2}{x^3} + \cdots,$$
$$\mu_n = \mathrm{B}(n+q, p-q+1) = \frac{\Gamma(n+q)\Gamma(p-q+1)}{\Gamma(n+p+1)} \tag{7}$$

The recurrence relation (2) is needed in various applications, whence the importance of getting the recurrence coefficients (Lanczos constants) from the moments μ_n (Schwarz constants, see [14] for these names). Some of our examples have been solved in the past, see the results in Table 1.

	(4) Legendre	(5) mod. Jacobi Chihara [13, chap. 5, § 2 (G)]	(7) Jacobi on $(0,1)$ Abramowitz [1, § 22.2.2, § 22.7.2]
a_n^2	$\dfrac{n^2}{4n^2-1}$	$\dfrac{2n+1-(-1)^n}{4(2n+1+(1)^n)}$	$\dfrac{n(n+p-1)(n+q-1)(n+p-q)}{(2n+p-2)(2n+p-1)^2(2n+p)}$
b_n	0	0	$\dfrac{2n(n+p)+q(p-1)}{(2n+p+1)(2n+p-1)}$

TABLE 1. Some known recurrence coefficients formulas.

General formulas for the recurrence coefficients from the power moments follow from the set of linear equations $\sum_0^{n-1}\mu_{i+j}c_j^{(n)} = -\mu_{i+n}, i = 0,\dots,n-1$ for the coefficients $c_j^{(n)}$ of $P_n(x) = x^n + \sum_0^{n-1} c_j^{(n)}x^j$, yielding $b_0+\cdots+b_{n-1} = -c_{n-1}^{(n)}$ and $\mu_0 a_1^2\cdots a_n^2 = D_{n+1}/D_n$, where D_n is the determinant of the stated set of equations (Hankel determinant). Various algorithms organize the progressive construction of the recurrence coefficients from the power moments but have an enormous condition number for large degree, whence the importance of alternate numerical methods [27], which will be considered in next section.

In some serendipitous cases, as seen in Table 1, closed-form formulas have been found [13, chapters 5 and 6] [60, § 18.3-18.37].

No formula is known for the dilogarithm case (6), and nothing simple must be expected, as the algorithm that follows produces the first a_n^2s which are $7/144, 647/11025,\dots$ and the first b_ns are $1/4, 13/28, 8795/18116,\dots$ [55].

2.2. **Asymptotic behaviour.**

Asymptotic behaviour of a_n and b_n has been enormously investigated. The simplest, and most meaningful, result is that, if the derivative $w=\mu'$ of the absolutely continuous[1] part is positive a.e. on (a,b), then

$$a_n \to a_\infty = \frac{b-a}{4}, \qquad b_n \to b_\infty = \frac{a+b}{2}, \qquad n\to\infty. \tag{8}$$

This seemingly simple result took decades to receive a complete proof, see the surveys by D.S. Lubinsky [48, §3.2], P. Nevai [57, §4.5], [58], and Van Assche's book [69, §2.6] for accurate statements and story.

A closer look to the Jacobi recurrence coefficients (7), Table 1 gives
$a_n = \dfrac{1}{4} - \dfrac{(q-1)^2+(p-q)^2-1/2}{16n^2} + o(n^{-2}), b_n = \dfrac{1}{2} + \dfrac{(q-1)^2-(p-q)^2}{8n^2} + o(n^{-2}).$

For a general interval (a,b), the Jacobi weight is $(b-x)^\alpha(x-a)^\beta$, and the relevant asymptotic behaviour is

$$a_n = \frac{b-a}{4}\left(1-\frac{\alpha^2+\beta^2-1/2}{4n^2}+o(n^{-2})\right), b_n = \frac{a+b}{2}+\frac{(b-a)(\alpha^2-\beta^2)}{8n^2}+o(n^{-2}). \tag{9}$$

This behaviour is thought to be present for all weights behaving like powers near the support's endpoints. Interior singularities create wilder oscillating perturbations, as it will be recalled later on. Lambin and Gaspard [43, Appendix] made interesting numerical tests on problems of solid-state physics by reducing the oscillating terms through sums and products, their formulas are:

[1] $d\mu = d\mu_{\text{absolutely continuous}} + d\mu_{\text{singular}}$.

$a_1 \cdots a_n = \text{const.} \left(\dfrac{b-a}{4}\right)^n \left(1 + \dfrac{\alpha^2+\beta^2-1/2}{4n} + o(1/n)\right)$,

$b_0 + \cdots + b_n = n\dfrac{a+b}{2} + \text{const.} - \dfrac{(b-a)(\alpha^2-\beta^2)}{8n} + o(1/n)$. I know no proof of the validity of these strong asymptotic estimates. Perturbation of a Jacobi weight is considered by Nevai and Van Assche [59, § 5.2]. See also L.Lefevre et al. [45] for more applications with Jacobi polynomials.

Other cases will be studied in §4.

3. Modified moments.

A very efficient technique for computing large numbers of recurrence coefficients is described here.

3.1. Main properties and numerical stability.

We consider a sequence of polynomials $\{R_0, R_1, \dots\}$ with R_n of degree n. Here, R_n need not be monic. The related modified moment of degree n is then

$$\nu_n = \int_a^b R_n(t)\, d\mu(t). \tag{10}$$

We want to compute the recurrence relation coefficients (2) from the modified moments of $d\mu$. The algebraic contents of the problem is the same as before, as each modified moment is a finite linear combination of the power moments, but the numerical accuracy in finite precision can be strongly enhanced: with the notation (f,g) for the scalar product $\int_a^b f(x)g(x)\, d\mu(x)$, we again compute the values $(P_n, R_j), n, j = 0, 1, \dots, N-1$ by

$$\begin{aligned}\boldsymbol{G}_N &= \begin{bmatrix} (R_0,R_0) & \cdots & (R_0,R_{N-1}) \\ \vdots & \vdots & \vdots \\ (R_{N-1},R_0) & \cdots & (R_{N-1},R_{N-1}) \end{bmatrix} \\ &= \begin{bmatrix} (R_0,P_0) & 0 & \cdots & 0 \\ (R_1,P_0) & (R_1,P_1) & \cdots & 0 \\ \vdots & & \ddots & \\ (R_{N-1},P_0) & (R_{N-1},P_1) & \cdots & (R_{N-1},P_{N-1}) \end{bmatrix} \begin{bmatrix} 1/\|P_0\|^2 & & & \\ & 1/\|P_1\|^2 & & \\ & & \ddots & \\ & & & 1/\|P_{N=1}\|^2 \end{bmatrix} \\ &\qquad \begin{bmatrix} (P_0,R_0) & (P_0,R_1) & \cdots & (P_0,R_{N-1}) \\ 0 & (P_1,R_1) & \cdots & (P_1,R_{N-1}) \\ & & \ddots & \vdots \\ 0 & 0 & \cdots & (P_{N-1},R_{N-1}) \end{bmatrix}\end{aligned} \tag{11}$$

In (11), the left-hand side is the Gram matrix of the basis $\{R_0, \dots, R_{N-1}\}$, which is factored as a lower triangular matrix times a diagonal matrix times an upper triangular matrix which happens to be the transposed of the first factor. The equation (11) is the matrix writing of the Gaussian (!) elimination method, also known for a positive definite matrix as Cholesky's method [8, 9]. See also Bultheel & Van Barel [11, § 4.2] for this connection of the Gram-Schmidt method with modified moments.

The numerical stability of the computation of the factors of the right-hand side of (11) is measured by the condition number of the matrix $\boldsymbol{G}_N$, which is the ratio of the extreme eigenvalues of the matrix (for a general nonsymmetric matrix, singular values must be considered [31,74]), after a convenient scaling replacing $R_n(x)$ by $R_n(x)/\rho_n$. The extreme eigenvalues are easily seen as the inf and sup on real vectors $[c_0, \dots, c_{N-1}]$ of the ratio $\dfrac{\sum_j \sum_k c_j c_k (R_j/\rho_j, R_k/\rho_k) = \int_a^b p^2(x)\, d\mu(x)}{\sum_j c_j^2}$, where $p(x) = \sum_j c_j R_j(x)/\rho_j$ (Rayleigh quotient [74, §54]). Now, in the important special case where the R_n/ρ_ns are the orthonormal polynomials with respect to a measure $d\mu_R$ with the same support as $d\mu$, the extreme eigenvalues are the inf and sup on the real polynomials p of degree $< N$ of $\dfrac{\int p^2(x)d\mu(x)}{\int_a^b p^2(x)d\mu_R(x)}$ so that these eigenvalues remain bounded and bounded from below if $d\mu(x)/d\mu_R(x)$ is similarly bounded.

3.2. **The algorithm.**

Stable and efficient computation of the recurrence coefficients of (2) from the modified moments (10) has been first published by Sack and Donovan in 1969 [64, 65], immediately enthusiastically commented and expanded by W. Gautschi [25] whose exposition is summarized here.

One does not compute the matrix of the left-hand side of (11) to get the orthogonal polynomials P_n. Instead, we use polynomials R_n satisfying themselves a known recurrence formula

$$xR_k(x) = A_kR_{k+1}(x) + B_kR_k(x) + \cdots + Z_kR_{k-s}(x), \tag{12}$$

containing the ordinary moments case when $s = 0$, some other (possibly formal) orthogonal polynomials when $s = 1$, and we shall even try an example where $s = 2$!
We make vectors $\boldsymbol{v}_n = [\int_a^b P_n(t)R_0(t)d\mu(t), \int_a^b P_n(t)R_1(t)d\mu(t), \ldots, \int_a^b P_n(t)R_{2N}(t)d\mu(t)]$, looking like the rows of the last factor of (11), for $n = 0, 1, \ldots, N-1$, starting of course with the modified moments at $n = 0$. We also define $\boldsymbol{v}_{-1}$ to be the null vector. Then, by (2) and (12),

$$\boldsymbol{v}_{n+1,k} = \int_a^b P_{n+1}(t)R_k(t)d\mu(t) = \int_a^b (t-b_n)P_n(t)R_k(t)d\mu(t)$$
$$- a_n^2\int_a^b P_{n-1}(t)R_k(t)d\mu(t) = \int_a^b [A_kR_{k+1}(t) + (B_k - b_n)R_k(t) + \cdots + z_kR_{k-s}(t)]P_n(t)d\mu(t)$$
$$- a_n^2\int_a^b P_{n-1}(t)R_k(t)d\mu(t)$$

using therefore elements of $\boldsymbol{v}_n$ and $\boldsymbol{v}_{n-1}$.

As one must have $\boldsymbol{v}_{n+1,n-1} = 0$, $a_n^2 = A_{n-1}\boldsymbol{v}_{n,n}/\boldsymbol{v}_{n-1,n-1}$ if $n > 0$ follows, and $\boldsymbol{v}_{n+1,n} = 0 \Rightarrow b_n = B_n + A_n\boldsymbol{v}_{n,n+1} - a_n^2\boldsymbol{v}_{n-1,n}$.

There will be much ado later on about the Chebyshev polynomials on $[a, b] : R_0(t) \equiv 1, R_1(t) = T_1((2t-a-b)/(b-a)) = (2t-a-b)/(b-a), R_2(t) = T_2((2t-a-b)/(b-a)) = 2((2t-a-b)/(b-a))^2 - 1, \ldots$ satisfying $tR_n(t) = (b-a)R_{n-1}(t)/4 + (a+b)R_n(t)/2 + (b-a)R_{n+1}(t)/4$. If we have a software allowing fast shift vector operations shiftleft($[a_1, \ldots, a_N]$) $= [a_2, \ldots, a_N, 0]$, shiftright($[a_1, \ldots, a_N]$) $= [0, a_1, \ldots, a_{N-1}]$, then
$\boldsymbol{v}_{n+1} = (b-a)[\text{shiftleft}(\boldsymbol{v}_n) + \text{shiftright}(\boldsymbol{v}_n)]/4 + (a+b)\boldsymbol{v}_n/2 - a_n^2\boldsymbol{v}_{n-1} - b_n\boldsymbol{v}_n$.

4. **Weights with logarithmic singularities.**

4.1. **Endpoint singularity.**

B. Danloy [16] considered the generation of orthogonal polynomials of degrees up to N related to $d\mu(x) = -\log x$ on $(0, 1)$ through the exact and stable computation of integrals $J(F) = -\int_0^1 F(x)\log x\, dx$ of some polynomials F of degree $\leqslant 2N-1$ by $J(F) = \int_0^1 x^{-1}G(x)dx$, where G is the integral of F vanishing at 0. If G is numerically available everywhere on $[0, 1]$, an $N-$point Legendre integration formula will do. As $G(x) = \int_0^x F(t)dt = x\int_0^1 F(xu)du$, another Legendre formula, x being now a known value, may be used for $G(x)$ itself.

This technique is probably close to using Legendre modified moments, with $R_n(x) =$ the Legendre polynomial of argument $2x-1$. From tables and formulas of Legendre polynomials [1, 60] etc., one has $R_0 = 1, R_1(x) = 2x-1, R_{n+1}(x) = [(2n+1)(2x-1)R_n(x) - nR_{n-1}(x)]/(n+1), R_n(0) =$

$(-1)^n, R_n(1) = 1, \|R_n\|_R^2 = \int_0^1 R_n^2(x)dx = 1/(2n+1)$. The integral of R_n is of special interest, it is $\int_0^x R_n(t)dt = (R_{n+1}(x) - R_{n-1}(x))/(2(2n+1))$ [21, p.157], whence the modified moments $\nu_0 = 1, \nu_n = -\displaystyle\int_0^1 R_n(t)\log t\,dt = \int_0^1 \frac{R_{n+1}(t) - R_{n-1}(t)}{2(2n+1)t}dt = -\int_0^1 \frac{R_n(t) + R_{n-1}(t)}{2(n+1)t}dt = \frac{(-1)^n}{n(n+1)}, n = 1, 2, \ldots$ [60, 14.18.6 Christoffel Darboux], also a special case of Jacobi polynomials formulas by Gautschi [28, eq. (16)]. It is then possible to compute safely thousands of recurrence coefficients:

n	an	n^2(1-4an)	bn	4n^2(1/2-bn)
1	0.220479275922	0.118082896312	0.464285714286	0.142857142857
2	0.242249473180	0.124008429112	0.485482446456	0.232280856701
3	0.246431702341	0.128458715707	0.492103081871	0.284289052631
4	0.247955681921	0.130836357052	0.495028498758	0.318176079465
8	0.249477328973	0.133803782828	0.498497801978	0.384562693567
16	0.249869046950	0.134095923477	0.499581244730	0.428805396441
32	0.249967482083	0.133193386867	0.499888698236	0.455892025643
64	0.249991945708	0.131961522042	0.499971199715	0.471863875255
128	0.249998004462	0.130779600850	0.499992656970	0.481232839609
256	0.249999504958	0.129772274044	0.499998142922	0.486821840702
512	0.249999877019	0.128954887187	0.499999532447	0.490264501879
1024	0.249999969410	0.128304217065	0.499999882584	0.492475910736
2048	0.249999992383	0.127788397553	0.499999970557	0.493964461229
4096	0.249999998102	0.127377905267	0.499999992624	0.495014502472
8192	0.249999999527	0.127048597789	0.499999998153	0.495787847453
16384	0.249999999882	0.126781755127	0.499999999538	0.496378968725
32768	0.249999999970	0.126563194895	0.499999999884	0.496844833204
65536	0.249999999993	0.126382258152	0.499999999971	0.497221088618

TABLE 2. Recurrence coefficients values and behaviour for logarithmic weight on $(0, 1)$.

As the weight function $-\log x$ vanishes at the upper endpoint, we certainly have $\alpha = 1$ in a comparison with the Jacobi weight $(1-x)^\alpha x^\beta$. With $\beta = 0$, one should have limit values $(\alpha^2 + \beta^2 - 1/2)/4 = 1/8$ and $(\alpha^2 - \beta^2)/2 = 1/2$, so $4a_n = 1 - \dfrac{1/2}{4n^2} + o(n^{-2}), b_n = \dfrac{1}{2} + \dfrac{1}{8n^2} + o(n^{-2})$, from (9) when $a = 0, b = 1$.

If convergence towards 1/8 and 1/2 holds in table 2, it must be extremely slow, values have been listed at powers of 2, in the hope of exhibiting a logarithmic behaviour. To be sure of the accuracy, computations were made with precision of 28 digits, and checked with a precision of 55 digits. The question will not be examined further here.

Quite another trend is given by known formulas for some multiple orthogonal polynomials, summarized here: the polynomial $R_n = R_{\{n_1,\ldots,n_p\}}$ of degree $n = n_1 + \cdots n_p$ is a multiple orthogonal polynomial with respect to the measures $d\mu_1, \ldots, d\mu_p$ if R_n is orthogonal to polynomials of degree $< n_1$ with respect to $d\mu_1$, of degree $< n_2$ w.r.t. $d\mu_2, \ldots$, of degree $< n_p$ w.r.t. to $d\mu_p$. This goes back to Hermite and Padé, and even to Jacobi (Jacobi-Perron algorithm), see [10]. An interesting recurrence relation (12) with $s = p$ occurs when[2] $n_j = 1 + \lfloor (n-j)/p \rfloor, j = 1, \ldots, p$.

Let $p = 2, d\mu_1(x) = x^{\alpha_1}dx$ and $d\mu_2(x) = x^{\alpha_2}dx$ on $(0, 1)$. The corresponding polynomials R_n are explicitly known [2]. As they are orthogonal to polynomials of degree $< \min(n_1, n_2)$ with respect to any linear combination with constant coefficients of $d\mu_1$ and $d\mu_2$, let us take α_1

[2]The floor $\lfloor x \rfloor$ = the largest integer $\leqslant x$.

and $\alpha_2 \to 0$, then the orthogonality holds with respect to the constant weight and the limit of $\dfrac{x^{\alpha_2} - x^{\alpha_1}}{\alpha_2 - \alpha_1}$ which is $\log x$, there we are: R_n does the half of the job, as it is orthogonal with respect to the logarithmic weight to polynomials of degree $< n/2$ if n is even, of degree $< (n-1)/2$ if n is odd. We have $R_n(x) = \dfrac{1}{n_1!\, n_2!} \dfrac{d^{n_2}}{dx^{n_2}} \left[x^{n_2} \dfrac{d^{n_1}}{dx^{n_1}} x^{n_1} (x-1)^n \right]$ [2, §3.3], symmetric in n_1 and n_2, $R_n(0) = (-1)^n, R_n(1) = \dfrac{n!}{n_1! n_2!}$, $R_0 = 1, R_1(x) = 2x - 1, R_2(x) = 9x^2 - 8x + 1, R_3(x) = 40x^3 - 54x^2 + 18x - 1, R_4(x) = 225x^4 - 400x^3 + 216x^2 - 36x + 1$, and the recurrence relation

$$\begin{aligned} xR_n(x) &= \frac{4(n+1)^2(n+2)}{(3n+2)^2(3n+4)} R_{n+1}(x) + \frac{4(n^2 + 19n/9 + 1)}{(3n+2)(3n+4)} R_n(x) \\ &\quad + \frac{4n(27n^2 - 16)}{9(3n-2)(3n+2)^2} R_{n-1}(x) + \frac{4n(n-1)}{3(3n-2)(3n+2)} R_{n-2}(x) \text{ if } n \text{ is even,} \\ &= \frac{4(n+1)}{9(3n+1)} R_{n+1}(x) + \frac{4(9n^2 - n - 1)}{9(3n-1)(3n+1)} R_n(x) + \frac{4n^2}{3(n+1)(3n+1)} R_{n-1}(x) \\ &\quad + \frac{4n(n-1)^2}{3(3n-1)(3n+1)(n+1)} R_{n-2}(x) \text{ if } n \text{ is odd.} \end{aligned} \tag{13}$$

The vectors of scalar products $\boldsymbol{v}_n = [(R_0, P_n), (R_1, P_n), \ldots]$ have only a finite number of nonzero elements from (R_n, P_n) to (R_{2n+1}, P_n).

```
v0 = [ 1 -1/2             0          0       0   0  0 ... ]
v1 = [ 0 7/72   -11/144   -1/40      0       0   0  0 ... ]
v2 = [ 0  0   647/25200   -3/175 -89/4900 -1/504 0  0 ... ]
```

Unfortunately, numerical stability for large n is poor, the amplification of the effects of rounding errors is about $2^{n/2}$ after n steps. This may be related to the behaviour of $|R_n(x)|$ on $[0,1]$, increasing from 1 to about 2^n instead of keeping an approximately equal ripple, as orthogonal polynomials do.

4.2. **Interior singularity: the Szegő asymptotic formula.**

The influence of an algebraic singularity at $c \in (a,b)$ on the recurrence coefficients has been discussed in [22, 49, 50], it has been observed, and sometimes proved, that

$$a_n - a_\infty = f_n \cos(2n\theta_c + \varphi_c) + o(f_n), b_n - b_\infty = 2f_n \cos((2n+1)\theta_c + \varphi_c) + o(f_n), \tag{14}$$

where $c = \dfrac{a+b}{2} + \dfrac{b-a}{2} \cos\theta_c$, with $0 < \theta_c < \pi$, $a_\infty = \dfrac{b-a}{4}, b_\infty = \dfrac{a+b}{2}$ from (8), and where f_n and φ depend on the kind of singularity.

For weak singularities when the weight function remains bounded and bounded from below by a positive number in a neighbourhood of the singular point,

$$w(x) \approx w(c) + \text{const.}|x-c|^\alpha, \alpha > 0, 0 < w(c) < \infty \Rightarrow f_n = \text{const.}n^{-\alpha-1}, \tag{15}$$

see [49, p.156], first part of [50].

When $w(c) = 0$ or ∞, the power of n in f_n does not depend on α, but we know

$$w(x) \sim \text{const.}|x-c|^\alpha, \alpha > -1 \Rightarrow f_n = -(b-a)|\alpha|/(8n), \tag{16}$$

[22, 50].

The discussion of these formulas depends on our knowledge of the asymptotic behaviour of the orthogonal polynomials of large degree. This description has been achieved by G. Szegő long ago, and is available of course in his book [67, chap. 12], also in the surveys by Lubinsky [48] and Nevai [57], and in Van Assche's book [69, §1.3.1] the formula for the orthonormal polynomial is

$$p_n(x) \approx (2\pi)^{-1/2}[z^n \exp(\lambda(z^{-1})) + z^{-n}\exp(\lambda(z))], \tag{17a}$$

where $x = b_\infty + 2a_\infty \cos\theta, z = e^{i\theta}$, and $\lambda(z) = \lambda_0/2 + \lambda_1 z + \lambda_2 z^2 + \cdots$ is a part of the Laurent-Fourier expansion $\log[w(x)\sqrt{(x-a)(b-x)}] = \log[2a_\infty w(b_\infty + 2a_\infty\cos\theta)|\sin\theta|] = -\sum_{-\infty}^{\infty}\lambda_k z^k = -\lambda(z) - \lambda(z^{-1})$ on $|z = e^{i\theta}| = 1$. The condition of validity is the minimal condition $\log[w(x))\sqrt{(x-a)(b-x)}] \in L_1$ (Szegő class). The function $D(z) = \exp(-\lambda(z))$ is the *Szegő function* associated to the weight w, it is analytic without zero in the unit disk, and satisfies $|D(z)|^2 \to w(x)\sqrt{(x-a)(b-x)}$ when $|z| \to 1$. Remark that the $\lambda_{-n} = \lambda_n$s are real. When $\exp(\lambda(z))$ is a polynomial of degree, say d, the formula (17a) is exact for $n > d/2$ (Bernstein-Szegő class). In the simplest case $w(x) = 1/\sqrt{(x-a)(b-x)}$, $p_n(x) = \sqrt{2/\pi}\cos n\theta = \sqrt{2/\pi}T_n((x-b_\infty)/(2a_\infty)), \lambda(z) \equiv 0$. For Chebyshev polynomials of the second kind, $w(x) = \sqrt{(x-a)(b-x)}$, $p_n(x) = \dfrac{\sin(n+1)\theta}{a_\infty\sqrt{2\pi}\,\sin\theta} = (1/\sqrt{2\pi})U_n((x-b_\infty)/(2a_\infty)), w(x)\sqrt{(x-a)(b-x)} = (x-a)(b-x) = 4a_\infty^2\sin^2\theta = -a_\infty^2(z-z^{-1})^2 = a_\infty^2(1-z^2)(1-z^{-2}), e^{\lambda(z)} = 1/[a_\infty(1-z^2)]$.

For the function of second kind $q_n(x) = \displaystyle\int_a^b \frac{p_n(t)\,dt}{x-t}$,

$$q_n(x) \approx (2\pi)^{1/2}\frac{4}{b-a}\,\frac{\exp(-\lambda(z^{-1}))}{z^n(z-z^{-1})}, \tag{17b}$$

see Barrett [3], also Van Assche [69, §5.4].

We also have $z = \cos\theta + i\sin\theta = (b-a)^{-1}[2x - a - b + 2\sqrt{(x-a)(x-b)}]$, with the square root such that $|z| > 1$ if $x \notin [a,b]$, in which case only the term containing z^n has to be considered in (17a). Remark that $x = b_\infty + a_\infty(z + 1/z) \Rightarrow z = (x - b_\infty)/a_\infty + O(1/x)$ when x is large, allowing to estimate the coefficients of x^n and x^{n-1}: let $p_n^{(0)}(x)$ and $q_n^{(0)}(x)$ be the right-hand sides of (17a)-(17b), then $p_n(x) \approx p_n^{(0)}(x) = \kappa_n^{(0)}x^n + \kappa_n'^{(0)}x^{n-1} + \cdots$, and

$$\kappa_n^{(0)} = \frac{\exp(\lambda_0/2)}{\sqrt{2\pi}\,(a_\infty)^n}, \quad \frac{\kappa_n'^{(0)}}{\kappa_n^{(0)}} = -nb_\infty + a_\infty\lambda_1. \tag{18}$$

Indeed, $p_n^{(0)}(x) == (2\pi)^{-1/2}z^n\exp(\lambda_0/2 + \lambda_1 z^{-1} + \lambda_2 z^{-2} + \cdots)$ and $z = x/a_\infty - b_\infty/a_\infty - a_\infty/x + O(x^{-2})$, so, the coefficient of x^n, $\kappa_n^{(0)} = (2\pi)^{-1/2}\exp(\lambda_0/2)/a_\infty^n$, and $z = x/a_\infty - b_\infty/a_\infty - a_\infty/x + O(x^{-2}) \Rightarrow p_n^{(0)}(x)/\kappa_n^{(0)} = (a_\infty z)^n\exp(\lambda_1 z^{-1} + \lambda_2 z^{-2} + \cdots) = (a_\infty z)^n + a_\infty\lambda_1(a_\infty z)^{n-1} + a_\infty^2(\lambda_1^2/2 + \lambda_2)(a_\infty z)^{n-2} + \cdots = x^n - (nb_\infty - a_\infty\lambda_1)x^{n-1} + \cdots$.

For the $p_n(x) = \kappa_n x^n + \kappa_n' x^{n-1} + \cdots$ itself, from the recurrence relation (2) $P_n(x) = p_n(x)/\kappa_n = (x - b_{n-1})P_{n-1}(x) - a_{n-1}^2 P_{n-2}(x)$, and $\|P_n\|^2 = \mu_0 a_1^2\cdots a_n^2$:

$$\kappa_n = \frac{1}{\sqrt{\mu_0}\,a_1\cdots a_n}, \frac{\kappa_n'}{\kappa_n} = -b_0 - \cdots - b_{n-1}. \tag{19}$$

Each term of (19) behaves like the corresponding term of (18) when $n \to \infty$.

In terms of z such that $x = a_\infty z + b_\infty + a_\infty/z$:

$$p_n(x)/\kappa_n = a_\infty^n z^n + a_\infty^{n-1}(nb_\infty - b_0 - \cdots - b_{n-1})z^{n-1} + \cdots \tag{20}$$

Quick and dirty check of (17a): $\displaystyle\int_a^b p_n(x)p_m(x)w(x)dx \approx \int_a^b p_n^{(0)}(x)p_m^{!0)}(x)w(x)dx$

$$= \frac{1}{2\pi}\int_a^b [z^n\exp(\lambda(z^{-1})) + z^{-n}\exp(\lambda(z))][z^m\exp(\lambda(z^{-1})) + z^{-m}\exp(\lambda(z))]\frac{\exp(-\lambda(z) - \lambda(z^{-1}))dx}{a_\infty|z - z^{-1}|}.$$

With $x = b_\infty + a_\infty(z+z^{-1}), dx = a_\infty(z-z^{-1})\dfrac{dz}{z}$, we have the integral on the unit circle $\dfrac{1}{4\pi i}\oint[z^{n+m}\exp(\lambda(z^{-1})-\lambda(z)) + z^{n-m} + z^{m-n} + z^{-n-m}\exp(\lambda(z)-\lambda(z^{-1}))]\dfrac{dz}{z}$. The central terms leave no residue if $m \neq n$. When $m = n$, the result is unity, together with perturbations involving high index Fourier coefficients of $\exp(\lambda(z)-\lambda(z^{-1}))$.

These high index coefficients enter the following estimate of recurrence coefficients finer asymptotics:

$$a_n - a_\infty \approx \frac{a_\infty}{2}(\psi_{-2n+2}-\psi_{-2n}), \quad b_n - b_\infty \approx a_\infty(\psi_{-2n+1}-\psi_{-2n-1}), \tag{21}$$

where the ψs are the Fourier coefficients of $\psi(e^{i\theta}) = \exp(\lambda(e^{-i\theta})-\lambda(e^{i\theta})) = \sum_{-\infty}^{\infty}\psi_k e^{ik\theta}$. This formula has been established by a long and painful proof through Toeplitz determinants in [49, p. 153, 158, 167] for weak singularities (the weight function w being continuous and bounded from below by a positive number at the singular point).

Remark that $\sum 2(a_n - a_\infty)z^{-2n} + (b_n - b_\infty)z^{-2n-1} \sim a_\infty \sum[\psi_{-k+2}z^{-k} - \psi_{-k}z^{-k}] =$ sum of negative exponents of z in $(z^{-2}-1)\psi(z)$.

Remark also that $\exp(\lambda(z^{-1})-\lambda(z)) = D(z)/D(z^{-1})$ in Szegő's notation, is an *inner function*, i.e., of modulus unity when $|z|=1$, so $\sum \psi_n\psi_{n+k} = \delta_{k,0}$.

An even stronger estimate follows from a refinement of the asymptotic matching of (18) and (19):

$$\sqrt{\frac{\mu_0 e^{\lambda_0}}{2\pi}}\,\frac{a_1\cdots a_n}{a_\infty^n} - 1 \sim -\frac{\psi_{-2n}}{2}, \quad b_0 + \cdots + b_{n-1} - nb_\infty + a_\infty\lambda_1 \sim -a_\infty\psi_{-2n+1}. \tag{22}$$

Can we find a quick and dirty argument for (21) and (22)?

Consider the square of the norm of the monic orthogonal polynomial $\mu_0 a_1^2\cdots a_n^2 = \|P_n\|^2 \approx \|P_n^{(0)}\|^2 = \int_a^b (p_n^{(0)}(t))^2 w(t)dt/(\kappa_n^{(0)})^2$ with $p_n^{(0)}$ being the right-hand side of (17a). We take a better look at the integral $\displaystyle\int_a^b (p_n^{(0)}(t))^2 w(t)dt = \frac{1}{4\pi i}\oint[z^{2n}\exp(\lambda(z^{-1})-\lambda(z)) + 2 + z^{-2n}\exp(\lambda(z)-\lambda(z^{-1}))]\frac{dz}{z} = 1 + \psi_{-2n}/2+$ the half of the coefficient of $\exp 2ni\theta$ of the complex conjugate $\overline{\psi(e^{i\theta})}$ which is $\psi_{-2n}/2$ again. We now need $\kappa_n^{(0)}$, already estimated in (18), but we need again a refined estimation. The coefficient of x^n of $p_n^{(0)}$ is estimated through the projection on the n^{th} degree element of an orthonormal basis of polynomials,so, by $p_n(x)$ times the scalar product of $p_n^{(0)}$ and the unknown p_n, which we replace by… $p_n^{(0)}$ (this part of the argument is very weak), and we get refined $\kappa_n^{(0)} =$ the $\kappa_n^{(0)}$ of (18) times the square of the norm of $p_n^{(0)}$, which is $1+\psi_{-2n}$ as seen above, and $\mu_0 a_1^2\cdots a_n^2 \approx \dfrac{2\pi\exp(-\lambda_0)(a_\infty)^{2n}}{1+\psi_{-2n}}$ follows, leading to the first part of (22). For the second part, see that $-b_0 - \cdots - b_{n-1}$ is the coefficient of x^{n-1} of $p_n(x)/\kappa_n \approx p_n^{(0)}(x)/\kappa_n^{(0)}$ estimated by its projections on p_n and p_{n-1} again replaced (same caution) by $p_n^{(0)}$ and $p_{n-1}^{(0)}$. Result is $-b_0 - \cdots - b_{n-1} \approx \kappa_n'^{(0)}/\kappa_n^{(0)} + (\kappa_{n-1}^{(0)}/\kappa_n^{(0)})$ times the scalar product of $p_n^{(0)}$ and $p_{n-1}^{(0)} = \dfrac{1}{4\pi i}\oint[z^{2n-1}\exp(\lambda(z^{-1})-\lambda(z)) + z + 1/z + z^{-2n+1}\exp(\lambda(z)-\lambda(z^{-1}))]\dfrac{dz}{z} = \psi_{-2n+1}$ as seen before in similar situations, and the second part of (22) follows.

This "proof" of (22) is terrible! It repeatedly confuses p_n and $p_n^{(0)}$, ignoring that $p_n^{(0)}$ is normally NOT a polynomial, so that various ways of estimating coefficients yield various results, of which the most convenient ones are kept. I even turned to some numerical tests to be sure, see the end of the present subsection.

An alternate source of knowledge is therefore most welcome: Van Assche gave in [70] a survey on how Case, Geronimo, and Nevai (and himself too, see [59]) investigated the relation between recurrence coefficients and weight function modification, by introducing a function $\phi(x) = \lim_{n\to\infty} \dfrac{(z-z^{-1})P_n(x)}{a_\infty^n z^{n+1}}$ outside $[a,b]$ for x, i.e., when $|z|>1$, and where $P_n(x)$ is the monic polynomial $p_n(x)/\kappa_n \sim \sqrt{2\pi}\ a_\infty^n e^{-\lambda_0/2} p_n(x)$, so that $\phi(x) = (1-z^{-2})\exp(\lambda(z^{-1})-\lambda_0/2) = 1+\lambda_1/z + (\lambda_1^2/2+\lambda_2-1)/z^2+\cdots$, and it is shown in [70] that

$$\phi(x) = 1 - \sum_0^\infty \left[\frac{b_n-b_\infty}{a_\infty z^{n+1}} + \frac{a_{n+1}^2-a_\infty^2}{a_\infty^2 z^{n+2}}\right]\frac{P_n(x)}{a_\infty^n} \tag{23}$$

valid for x up to the sides of the cut $[a,b]$ in the trace-class case ($\sum_1^\infty |a_n-a_\infty|+|b_n-b_\infty|<\infty$).

Check Chebyshev polynomials of the first kind: $\lambda(z^{-1})\equiv 0$, $\phi(x) = \lim(z-z^{-1})[2T_n(x) = z^n+z^{-n}]/z^{n+1} = 1-z^{-2}$, OK, as only $a_1^2 = 2a_\infty^2$ is different from a_∞^2; Chebyshev polynomials of second kind: $\lambda(z)+\lambda(z^{-1}) = -\log(1-(z+z^{-1})^2/4), \lambda(z) = \log 2-\log(1-z^2)$, $\phi(x) = \lim(z-z^{-1})[U_n(x) = (z^{n+1}-z^{-n-1})/(z-z^{-1})]/z^{n+1} = 1$.

Can we extract from (23) information on $F(z) = \sum_0^\infty \left[\dfrac{b_n-b_\infty}{a_\infty z^{2n+1}} + \dfrac{a_{n+1}^2-a_\infty^2}{a_\infty^2 z^{2n+2}}\right]$?

From (17a) and (18), $P_n(x)/(a_\infty z)^n = p_n(x)/(\kappa_n a_\infty^n z^n)$ contains a part with strongly negative powers of z which tend to be close to the corresponding part of $\exp(\lambda(z)-\lambda_0/2)z^{-2n}$, and the corresponding part of $\sum_0^\infty \left[\dfrac{b_n-b_\infty}{a_\infty z} + \dfrac{a_{n+1}^2-a_\infty^2}{a_\infty^2 z^2}\right]\dfrac{P_n(x)}{a_\infty^n z^n}$, so, $(1-z^{-2})\exp(\lambda(z^{-1})-\lambda_0/2)$ $\approx 1-e^{-\lambda_0/2}\ \sum_0^\infty \left[\dfrac{b_n-b_\infty}{a_\infty} z^{-n-1} + \dfrac{a_{n+1}^2-a_\infty^2}{a_\infty^2} z^{-n-2}\right][z^n\exp(\lambda(z^{-1})) + z^{-n}\exp(\lambda(z))]$, or, after division by $e^{\lambda(z)-\lambda_0/2}$, $(1-z^{-2})\psi(z) \approx e^{\lambda_0/2-\lambda(z)} - \sum_0^\infty \left[\dfrac{b_n-b_\infty}{a_\infty} z^{-1} + \dfrac{a_{n+1}^2-a_\infty^2}{a_\infty^2} z^{-2}\right]\psi(z) -$ $\sum_0^\infty \left[\dfrac{b_n-b_\infty}{a_\infty} z^{-2n-1} + \dfrac{a_{n+1}^2-a_\infty^2}{a_\infty^2} z^{-2n-2}\right]$. This confirms that the latter series is related to the negative powers part of $\psi(z)$ precisely as stated in (21) .

An interesting exercise is also to recover (17a-17b) from (21) by working a linearization of a product of 2×2 matrices containing the recurrence coefficients: $\begin{bmatrix} p_{N-1}(x) & q_{N-1}(x) \\ p_N(x) & q_N(x)\end{bmatrix}$ $= \prod_{n=0}^{N-1} \begin{bmatrix} 0 & 1 \\ -a_{N-1-n}/a_{N-n} & (x-b_{N-1-n})/a_{N-n}\end{bmatrix}$ times $\begin{bmatrix} 0 & \sqrt{\mu_0}/a_0 \\ 1/\sqrt{\mu_0} & S(x)/\sqrt{\mu_0}\end{bmatrix}$ ([54]), and we use $(A+E_{N-1})(A+E_{N-2})\cdots(A+E_0) \approx A^N + \sum_{n=0}^{N-1} A^{N-1-n}E_nA^n$, seeing that $A = \begin{bmatrix} 0 & 1 \\ -1 & (x-b_\infty)/a_\infty\end{bmatrix} =$ $\begin{bmatrix} 1 & 1 \\ z & z^{-1}\end{bmatrix}\begin{bmatrix} z & 0 \\ 0 & z^{-1}\end{bmatrix}\begin{bmatrix} 1 & 1 \\ z & z^{-1}\end{bmatrix}^{-1} = U\ \mathrm{diag}(z,z^{-1})U^{-1}$, where $z+z^{-1} = (x-b_\infty)/a_\infty$, so that $A^{N-1-n}E_nA^n = U\ \mathrm{diag}(z^{N-1-n}, z^{-N+1+n})U^{-1}E_nU\ \mathrm{diag}(z^n,z^{-n})U^{-1}$ and we find $U^{-1}E_nU \approx (z^{-1}-z)^{-1}\begin{bmatrix} e_n(z) & e_n(z^{-1}) \\ -e_n(z) & -e_n(z^{-1})\end{bmatrix}$, where $e_n(z) = [(a_{n+1}-a_\infty)z^2 + (b_n-b_\infty)z + a_n - a_\infty]/a_\infty$, so that off-diagonal elements of the sum are $z^{\pm(N-1)}\sum z^{\mp 2n}e_n(z^{\mp 1})$ containing again the sum $\sum 2(a_n-a_\infty)z^{\mp 2n} + (b_n-b_\infty)z^{\mp(2n+1)}$.

It seems here that much energy has been spent on incomplete proofs, and that somebody should achieve a decent one!

Here is a test of the numerical credibility of (21), actually of the first part of (22): with $w(x) = (1-x^2)^{-1/2}\exp(|x|)$ on $(-1,1)$, $\lambda(e^{i\theta})+\lambda(e^{-i\theta}) = -|\cos\theta|$, $\lambda_{2n} = 2(-1)^n/((4n^2-1)\pi), \lambda(z) =$

$(2/\pi)(-1/2 - z^2/3 + z^4/15 - \cdots) = -(1+z^2)\dfrac{1}{2\pi i z}\log\dfrac{1+iz}{1-iz} = i\pi^{-1}\cos\theta\log[i\cot(\pi/4+\theta/2)]$ on $|z = e^{i\theta}| = 1$, actually $\cos\theta[-1/2 + i\pi^{-1}\log\cot(\pi/4+\theta/2)]$ when $-\pi/2 \leqslant \theta \leqslant \pi/2, \cos\theta[1/2 + i\pi^{-1}\log\cot(-\pi/4+\theta/2)]$ when $\pi/2 \leqslant \theta \leqslant 3\pi/2 : \lambda(e^{-i\theta}) - \lambda(e^{i\theta}) = 2i\pi^{-1}\cos\theta\log\cot(\pm\pi/4+\theta/2)$. Check that $\lambda(e^{-i\theta}) + \lambda(e^{i\theta}) = -|\cos\theta|$.

With $M_0 = \sqrt{\mu_0\exp(\lambda_0)/(2\pi)}$, the product $M_n = M_0 a_1 \cdots a_n/a_\infty^n \to 1$. Here, $\mu_0 = \int_{-1}^{1} w(t)dt = 6.2088, \lambda_0 = -0.63662, M_0 = 0.72306$, some a_n, λ_n, ψ_n are shown, and $2M_n - 2$ shows how M_n is close to $1 - \psi_{-2n}/2$ according to (22).

n	0	1	2	3	4	5	6	7	8	9	10
a_n		0.77414	0.43434	0.52081	0.49034	0.50548	0.49649	0.50243	0.49822	0.50136	0.49893
λ_{2n}	-0.63662	-0.21221	0.042441	-0.01819	0.01011	-0.00643	0.00445	-0.00327	0.00250	-0.00197	0.00160
ψ_{2n}	0.95317	0.21745	-0.022831	0.01252	-0.00738	0.00489	-0.00349	0.00262	-0.00204	0.00163	-0.00134
ψ_{-2n}	0.95317	-0.19755	0.058329	-0.02507	0.01353	-0.00838	0.00566	-0.00407	0.00306	-0.00238	0.00191
$2M_n - 2$		0.23899	-0.055036	0.02590	-0.01325	0.00851	-0.00559	0.00411	-0.00304	0.00240	-0.00189

TABLE 3. Results for $e^{|t|}/\sqrt{1-t^2}$.

4.3. **Relation with Fourier coefficients asymptotics.**

The main influence of a singularity at $\theta = \theta_c$ on the Fourier coefficient $\int_{-\pi}^{\pi} f(\theta)\exp(in\theta)d\theta$ of a function f is $\exp(in\theta_c)\hat{f}(n/(2\pi))$, see Lighthill [46, p.43, p.72], where $\hat{f}$ is the Fourier transform of f. An algebraic singularity of the form $|\theta - \theta_c|^\alpha$ is shown to correspond to an $n^{-\alpha-1}$ behaviour. This case is also given with much detail by A. Erdélyi [20, §2.8], and Zygmund [78, chap. 5, §2.24]. The nature of a weak singularity $w(c) +$ cont. $|x-c|^\alpha$ with $0 < w(c) < \infty$, is left unchanged by taking logarithms or exponentials, also in conjugate functions [78, chap.5, §2.6 and 2.24], so, the $1/n^{\alpha+1}$ is kept unchanged up to the ψ_ns and (15) is confirmed.

Stretching the argument for weak singularity to a strong singularity such as $w(t) \sim$ const. $|t-c|^\alpha$ near c, the logarithm of w behaves like $\alpha\log|\cos\theta - \cos\theta_c| =$ const. $+\alpha$ Re $\log(1 - e^{i\theta}/z_c)(1 - e^{-i\theta}/z_c)$ whence $\lambda_n \sim -\alpha$ Re $z_c^{-n}/n = -\alpha\cos(n\theta_c)/n, \lambda(z) \sim (\alpha/2)\log((1 - ze^{i\theta_c})(1 - ze^{-i\theta_c})) = (\alpha/2)\log(2e^{i\theta}(\cos\theta - \cos\theta_c))$ on the circle. Keeping logarithms of positive numbers to be real, $\lambda(e^{i\theta}) \sim (\alpha/2)[\log 2 + i\theta + \log(\cos\theta - \cos\theta_c)]$ when $-\theta_c < \theta < \theta_c$, $(\alpha/2)[\log 2 + i\theta - i\pi + \log(\cos\theta_c - \cos\theta)]$ otherwise. Then, $\lambda(e^{-i\theta}) - \lambda(e^{i\theta}) \sim -i\alpha\theta$ on the first arc, $i\alpha(\pi - \theta)$ on the second arc, and its exponential has $\psi_n = (2\pi)^{-1}[\int_{-\theta_c}^{\theta_c}\exp(-i(n+\alpha)\theta)d\theta + \exp(i\alpha\pi)\int_{\theta_c}^{2\pi-\theta_c}\exp(-i(n+\alpha)\theta)d\theta] = \dfrac{2}{\pi}\dfrac{\sin(\alpha\pi/2)\cos(n\theta_c + \alpha(\theta_c - \pi/2))}{\alpha + n}$ showing an $1/n$ asymptotic behaviour, but the amplitude is not right, it should have been $-a_\infty|\alpha|/2$ from (16).

And what about a logarithmic singularity, as encountered with 2−dimensional crystals?

Let $w(x) - A\log|x-c|$ be continuous in a neighbourhood of $c \in (a,b)$.

4.4. **Conjecture.** *If the weight function has one or several logarithmic singularities of the form $w(x) \sim$ const. $\log|x-c|$ near one or several values of $c \in (a,b)$, the main asymptotic behaviour of the related amplitude in* (14) *is*

$$f_n = \frac{(b-a)\sin\theta_c}{8n\log n}, \tag{24}$$

where $c = (a + b + (b-a)\cos\theta_c)/2$.

One has also $(b-a)\sin\theta_c = 2\sqrt{(c-a)(b-c)}$.

Now, $\log w(t)$ has a $\log\log$ singularity! There is probably not much literature on Fourier coefficients of a $\log(\log|t-c|)$ singularity, but Zygmund [78, chap. 5, §2.31], and Wong & Lin [75] show how to arrive at a $n^{-m-1}(\log n)^{\beta-1}$ from a $|t-c|^m(\log|t-c|)^\beta$ singularity, when m is an integer. Take $m=0$ and $\beta\to 0$, as $\log(\log|t-c|)$ is the limit when $\beta\to 0$ of $\beta^{-1}[(\log|t-c|)^\beta-1]$, we may expect the $1/n\log n$ of the conjecture. Two meaningful examples will be considered in § 7.

4.5. **Relation between jumps and logarithmic singularities.**

The Fourier series conjugate to the real part of $\sum c_k e^{ik\theta}$ is the imaginary part of the same expansion [78, § 1]. Jumps and logarithmic singularities are conjugate phenomena. A simple demonstration is given by the real part of $\log(1-z/e^{i\theta_c}) = -\sum_1^\infty e^{ik(\theta-\theta_c)}/k$ when $z=e^{i\theta}$. When $|z|<1$ and z close to $e^{i\theta}$, $1-z/e^{i\theta_c}$ is almost pure imaginary, and the complex logarithm is about $i\pi/2+\log|\theta-\theta_c|$ when $\theta<\theta_c$, and $-i\pi/2+\log|\theta-\theta_c|$ otherwise, so, a logarithm in the real part corresponds to a jump in the imaginary part, and these two kind of singularities create similar asymptotic behaviours in the Fourier coefficients, maybe the work done for a jump [23] can be the basis for a proof of the conjecture 4.4.

Unfortunately, the loose considerations of the preceding subsection suggest to look at the logarithm of the weight function. If the logarithm of a jump (between two positive values) is still a jump, log(log) is something new.

5. Expansions in functions of the second kind.

We proceed with modified moments and related expansions. The weight function w is not always given in such an explicit form allowing a fast way to compute the modified moments. It is often better to use the generating function $S(x)$ of the power moments, but how is $S(x)$ an expansion involving modified moments?

From now on, we choose R_n to be an orthogonal polynomial of degree n with respect to a weight function w_R on $[a,b]$, and the searched P_n orthogonal with respect to the weight function w so that $d\mu(x)=w(x)dx$. We will often need the ratio w/w_R, a writing more realistic than the Radon-Nykodim derivative $d\mu/d\mu_R$ in most cases.

We saw that the Laurent expansion of the Stieltjes function of w with the power moments is $S(x)=\int_a^b w(t)(x-t)^{-1}dt=\sum_0^\infty \mu_k\, x^{-k-1}$. See here the expansion involving the modified moments $\nu_n=\int_a^b R_n(t)\,w(t)\,dt$:

5.1. **Theorem.** *Let R_n, $n=0,1,\dots$ be orthogonal polynomials related to a weight w_R on $[a,b]$, with $\|R_n\|_R^2=\int_a^b R_n^2(t)\,w_R(t)\,dt$, and $S(x)=\int_a^b(x-t)^{-1}w(t)dt$ be the Stieltjes function of the weight function w. Then,*

$$S(x)=\sum_0^\infty \frac{\nu_n}{\|R_n\|_R^2}Q_n(x), \tag{25}$$

for $x\notin[a,b]$, where ν_n is the modified moment $\int_a^b R_n(t)\,w(t)\,dt$, and where $Q_n(x)=\int_a^b(x-t)^{-1}R_n(t)\,w_R(t)\,dt$ is the n^{th} function of the second kind related to the weight w_R.

Indeed, as R_n is a finite linear combination of powers, which may be inverted as $t^k=\sum_{n=0}^k c_{n,k}R_n(t)$, we have $S(x)=\sum_{k=0}^\infty\int_a^b t^k\,w(t)\,dt\,x^{-k-1}=\sum_{k=0}^\infty\int_a^b[\sum_{n=0}^k c_{n,k}R_n(t)]\,w(t)\,dt\,x^{-k-1}$ $=\sum_{n=0}^\infty \nu_n[\sum_{k=n}^\infty c_{n,k}x^{-k-1}]$.

Remark now the Laurent expansion $Q_n(x)=\sum_{k=n}^\infty\int_a^b t^k R_n(t)\,w_R(t)\,dt\,x^{-k-1}=\sum_{k=n}^\infty c_{n,k}\|R_n\|_R^2\,x^{-k-1}$. □

There is no convergence problem, at least if a and b are finite, as the Laurent expansions converges exponentially fast when $|x|>\max(|a|,|b|)$.

My first idea was to expand the ratio w/w_R in the $\{R_n\}$ basis, by $w(t)/w_R(t)$ $= \sum_{n=0}^{\infty}[\int_a^b (w(u)/w_R(u))w_R(u)R_n(u)dt = \nu_n]R_n(t)/\|R_n\|_R^2$ for t almost everywhere in $[a,b]$, but we do not need to discuss the validity of this expansion. It seems however strange that the theorem seems to be true in some eerie situations where w and w_R have different supports. The price is that the modified moments are unusually large, which make them completely useless. This is obvious if the support of w is bigger than the support of w_R, as the R_ns are free to become large outside the support of w_R. But things are not better if the support of w is too small! Recall that the condition number of the Gram matrix $\boldsymbol{G}_N$ in (11) depends also on the smallest eigenvalue, which is the infimum on polynomials p of degree $< N$ of the Rayleigh ratio $\int_a^b p^2 w\,dx / \int_a^b p^2 w_R\,dx$, and we may choose p to be very small on the part of (a,b) which is the support of w. See also Beckermann & Bourreau [4].

Expansions with functions of the second kind share properties of Laurent expansions, such as exponential speed of convergence outside $[a,b]$, and orthogonal expansions, such as the use of recurrence relations, see Barrett [3], Gautschi [26].

For Legendre functions, the connection between Laurent expansions and expansions in functions of the second kind is given by Heine's formula $(x-t)^{-1} = \sum_0^\infty (2m+1)P_m(t)Q_m(x), -1 < t < 1, x \notin [-1,1]$ (NIST [60, § 14.28.2], etc.), so that, gathering the t^n terms,
$\dfrac{1}{x^{n+1}} = \displaystyle\sum_0^n \dfrac{d^n P_m(0)/dt^n}{n!} Q_m(x)$, showing how the Q_n expansion is a rearrangement of the Laurent expansion.

As a matter of fact, the Heine's series is valid for any choice of orthogonal polynomials: expand $(x-t)^{-1}$ in orthogonal expansion of the R_ns:

$$\frac{1}{x-t} = \sum_{m=0}^{\infty} \frac{\displaystyle\int_a^b \frac{R_m(u)\, w_R(u) du}{x-u} = Q_m(x)}{\|R_n\|_R^2} R_m(t)$$

The subject matter will now be strongly simplified by turning to the Chebyshev case:

5.2. **Chebyshev functions of the second kind.** *The functions of second kind related to the Chebyshev polynomials* $R_n(x) = T_n((2x-a-b)/(b-a))$ *are*

$$Q_n(x) = \int_a^b \frac{T_n((2t-a-b)/(b-a))\, dt}{(x-t)\sqrt{(t-a)(b-t)}} = \frac{\pi}{a_\infty z^n (z-1/z)}, \tag{26}$$

[17, § 1.13], *where* $z = [2x-a-b+2\sqrt{(x-a)(x-b)}]/(b-a) \sim 4x/(b-a) = x/a_\infty$ *for large* $|x|$.

Indeed, we recalled in section 2.1 that the recurrence relations (2) are valid for the Q_ns. So, $Q_{n+1}(x) = 2(2x-a-b)Q_n(x)/(b-a) - Q_{n-1}(x) = (z+1/z)Q_n(x) - Q_{n-1}(x)$ for $n = 1,2,\ldots$ meaning that $Q_n(x)$ is a combination of z^{-n} and z^n, but boundedness for large x allows only z^{-n}. Finally, with $t = (a+b)/2 + ((b-a)/2)\cos\theta = b_\infty + 2a_\infty \cos\theta$, $Q_0(x) = \int_0^\pi d\theta/(x - b_\infty - 2a_\infty\cos\theta) = \int_0^\pi d\theta/(a_\infty(z+z^{-1}-2\cos\theta)) = \dfrac{1}{2i}\displaystyle\oint \dfrac{de^{i\theta}}{a_\infty(z-e^{i\theta})(e^{i\theta}-z^{-1})} = \dfrac{\pi/a_\infty}{z-z^{-1}}$, as only the residue at $e^{i\theta} = z^{-1}$ is to be considered, as $|z| > 1$.

When $x = b_\infty + 2a_\infty\cos\theta \pm i\varepsilon$ is close to $[a,b]$, the formula (26) turns to a finite part (Hilbert transform) added to $\pm\pi i T_n(\cos\theta)/\sqrt{(x-a)(b-x)}$ (Sokhotskyi-Plemelj [39, §14.1]). The finite part is known to be $-(\pi/(2a_\infty))U_{n-1}(\cos\theta)$ [1, 22.13.3], [52, eq. 9.22a], also used by Weisse & al. [73, eq. (14)]. It is also recalled that the asymptotic formula (17b) is exact in the Bernstein-Szegő case (when $\sqrt{(t-a)(b-t)}/w(t)$ is a polynomial, and when $n >$ half the degree of this polynomial). Henrici gives (26) in [39, § 14.6, Problem 2] with the symbol "U_n" for our Q_n.

5.3. **Corollary.** *Chebyshev modified moments are the coefficients of the expansion of the Stieltjes function in negative powers of* z

$$\frac{(b-a)(z-z^{-1})}{2} S\left(x = \frac{a+b}{2} + \frac{(b-a)(z+z^{-1})}{4}\right) = 2\nu_0 + \sum_1^\infty \frac{4\nu_n}{z^n}. \tag{27}$$

Indeed, put (26) in (25)

$$S(x) = \sum_0^\infty \frac{\nu_n}{\|R_n\|_R^2} Q_n(x) = \frac{\nu_0}{\|R_0\|_R^2 = \pi} \frac{\pi/a_\infty}{z - z^{-1}} + \sum_1^\infty \frac{\nu_n}{\|R_n\|_R^2 = \pi/2} \frac{\pi/a_\infty}{z^n(z-z^{-1})}. \qquad \square$$

6. About matrices in solid-state physics.

6.1. Matrix approximation of the Hamiltonian operator.

A solid-state system is a stable arrangement of atoms (whose positions are the *sites*) which may create, or at least amplify, interesting physical phenomena, such as electrical conductivity or magnetic field intensity. The relevant Hamiltonian is an operator acting on functions (the *states*) of three space variables, i.e. of a subset of $L^2(\mathbb{R}^3)$. This formidable set of functions[3] is approximated by linear combinations of a finite set of simple functions with a small support around each site, quite similar to finite elements constructions.

The kinetic part of the Hamiltonian involves the Laplace operator whose discretization about a site is the site value subtracted from the average of the values on neighbouring sites (a harmonic function at a point is the average on a surface about the point; after discretization, this integral average turns as a simple arithmetic mean of values at neighbouring points, this suggests why the discretized Laplacian involves an arithmetical mean); the potential part is also represented by a combination of nearby values (closest neighbour approximation, or tight-binding approximation see Economou's book [19, §5.2]) also the first pages of Giannozzi & al. [30] and Haydock [35,36]). Consider for instance a one-dimensional chain of sites $\{\dots, x_{n-1}, x_n, x_{n+1}, \dots\}$ at distance $x_{n+1} - x_n = \ell$ from each neighbour. The Laplace operator at x_n is the discretized second derivative = the divided second difference $\Delta^2 x_n/\ell^2 = (x_{n+1} - 2x_n + x_{n-1})/\ell^2$. Multiply by appropriate physical parameters, and add the potential of simple interactions between close neighbours and we have

$$H = \begin{bmatrix} \ddots & \ddots & \ddots & & & & \\ & \alpha & \beta & \alpha & & & \\ & & \alpha & \beta & \alpha & & \\ & & & \alpha & \beta & \alpha & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix} \tag{28}$$

The Hamiltonian operator is therefore represented by a huge sparse symmetric matrix where each row is associated to a site and contains a small number of nonzero elements corresponding to neighbouring sites (tight-binding approximation). A simple substance made of identical elements (pure crystal) will show the repetition of the same pattern in the matrix (Toeplitz matrix, in mathematicians lingo). Random modifications (doping) may of course be considered too. The study of these various configurations is of enormous interest in physical and technological applications [12, 18, 42, 44].

6.2. Density of states.

Let $\boldsymbol{u}$ be an initial state vector describing an electron on some site, i.e. only one element of $\boldsymbol{u}$ is nonzero. The time dependence of such a state vector shows how the electron diffuses on the other sites, starting with the close neighbours as expected [35, p. 217]. The equation is $\partial\boldsymbol{u}/\partial t =$

[3] And this is only for a single-electron operator, or we should have to consider a power of $L^2(\mathbb{R}^3)$.

$(i/\hbar)\boldsymbol{H}\boldsymbol{u}$ [35, §34], so $\boldsymbol{u}(t) = \exp((it/\hbar)\boldsymbol{H})\boldsymbol{u}(0)$, and we use eigenvalues and eigenstates $(E_p, \boldsymbol{v}^{(p)})$ of the simplified Hamiltonian operator. We now have $\boldsymbol{u}(t) = \sum_p \exp(itE_p/\hbar)(\boldsymbol{v}^{(p)}, \boldsymbol{u}(0))\boldsymbol{v}^{(p)}$ We consider the projection on the m^{th} site starting from the n^{th} site, and rearrange the sum as $\int_a^b \exp(itE/\hbar)d\mathcal{N}_{m,n}(E)$, where $\mathcal{N}_{m,n}(E)$ is a staircase function discontinuous at each eigenvalue. When $n = m$, $d\mathcal{N}_{n,n}(E)$ is the sum of the positive terms $|(\boldsymbol{v}^{(p)}, \boldsymbol{u}(0)|^2$ for the eigenvalues E_p in an interval of length dE around E (sorry for such a sloppy, pre-modern, use of infinitesimals). The result $n_{n,n}(E)dE$, where $n_{n,n}(E)$ is called the (local) *density of states*. In the example (28), the eigenvalues are $\beta + 2\alpha\cos(k\pi/N)$ if the matrix has N rows & columns; normalized eigenvectors are $\sqrt{2/N}\ \sin(mk\pi/N)$ (average value of the sine squares is 1/2), see [32, chap. 7], [35, §12] . If $a = \beta - 2\alpha < E < b = \beta + 2\alpha$, let $E = \beta + 2\alpha\cos\theta_E$, then, between E and $E + dE$, there are $(N/\pi)|\theta_{E+dE} - \theta_E|$ eigenvalues, to multiply by the average of the squares of eigenvector elements, what remains is $\pi^{-1}\left|\arccos\left(\dfrac{E+dE-\beta}{2\alpha}\right) - \arccos\left(\dfrac{E-\beta}{2\alpha}\right)\right| \approx \dfrac{dE}{\pi\sqrt{4\alpha^2-(E-\beta)^2}}$.

Nobody indulges in such awkward ways! Instead, one considers the *Green functions* [19, 30, 34–36] $G_{m,n}(x) = \displaystyle\int_a^b \frac{n_{m,n}(t)\,dt}{x-t} = ((x\boldsymbol{I} - \boldsymbol{H})^{-1})_{m,n}$, which, if $m = n$, have the properties of the Stieltjes functions of the first section!

6.3. **The recursion (Lanczos) method.**

Let $\boldsymbol{u}_0$ be a state represented by a vector of $\mathbb{R}^N$, and $\mu_n = (\boldsymbol{u}_0, \boldsymbol{H}^n\boldsymbol{u}_0)$, where (,) is the usual scalar product of $\mathbb{R}^N$. From the expansion of $\boldsymbol{u}_0$ in the orthonormal set of eigenstates $\{\boldsymbol{v}^{(p)}\}$ as seen above, $\mu_n = \sum_p E_p^n|(\boldsymbol{u}_0, \boldsymbol{v}^{(p)})|^2 = \int_a^b t^n d\mu(t)$, where $d\mu(t)$ is the relevant density of states times dt. As $\boldsymbol{H}$ is a very sparse matrix, the vectors $\boldsymbol{H}^n\boldsymbol{u}_0$ are easy to compute and they may be rearranged in an orthonormal sequence $\boldsymbol{u}_n = p_n(\boldsymbol{H})\boldsymbol{u}_0)$ by linear algebra constructions. Of course, this means that $\delta_{m,n} = (\boldsymbol{u}_m, \boldsymbol{u}_n) = (p_m(\boldsymbol{H}\boldsymbol{u}_0), p_n(\boldsymbol{H})\boldsymbol{u}_0) = (\boldsymbol{u}_0, p_m(\boldsymbol{H})p_n(\boldsymbol{H})\boldsymbol{u}_0)$ (from symmetry of $\boldsymbol{H}$) $= \int_a^b p_m(t)p_n(t)d\mu(t)$, so $p_n = \kappa_n P_n$ is the orthonormal polynomial of degree n with respect to $d\mu$. Therefore, from the recurrence relation $tp_n(t) = a_np_{n-1}(t) + b_np_n(t) + a_{n+1}p_{n+1}(t)$, $\boldsymbol{H}p_n(\boldsymbol{H}) = a_np_{n-1}(\boldsymbol{H}) + b_np_n(\boldsymbol{H}) + a_{n+1}p_{n+1}(\boldsymbol{H})$, or $\boldsymbol{H}\boldsymbol{u}_n = a_n\boldsymbol{u}_{n-1} + b_n\boldsymbol{u}_n + a_{n+1}\boldsymbol{u}_{n+1}$:

$$\boldsymbol{H}[\boldsymbol{u}_0 \mid \boldsymbol{u}_1 \mid \boldsymbol{u}_2 \mid \cdots] = [\boldsymbol{u}_0 \mid \boldsymbol{u}_1 \mid \boldsymbol{u}_2 \mid \cdots]\begin{bmatrix} b_0 & a_1 & & & \\ a_1 & b_1 & a_2 & & \\ & a_2 & b_2 & a_3 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{29}$$

so that the Hamiltonian matrix and the tridiagonal matrix of the recurrence coefficients have the same spectrum (should we be able to build N vectors $\boldsymbol{u}_n$s). From $\boldsymbol{u}_{n-1}$ (if $n > 0$) and $\boldsymbol{u}_n$, one gets a_n and b_n by $a_n = (\boldsymbol{u}_{n-1}, \boldsymbol{H}\boldsymbol{u}_n), b_n = (\boldsymbol{u}_n, \boldsymbol{H}\boldsymbol{u}_n)$ [27, § 3.1.7.1] [31, chap. 9].

The recursion method has been, and still is, quite an inspiration in solid-state physics! [24, 30, 35–37]. The Hamiltonian operator of a given physical system is approximated by a matrix $\boldsymbol{H}$ as above, and a set of recurrence coefficients is produced by the Lanczos method. The features of the weight function are then "read" from the asymptotic behaviour of these recurrence coefficients.

The reverse procedure is used here: from the known densities of states of model systems, the recurrence coefficients are produced through modified moments, and asymptotic properties are investigated.

6.4. **Pure crystals.**

The simplest pure crystal is a $d-$dimensional set of identical atoms related in the same way to their neighbours. If there is a large but finite number of atomic positions (sites), the Hamiltonian operator is a large matrix acting on a vector $v(x_1,\dots,x_d)$ as Hv at the available site $(x_1,\dots,x_d) = \sum_m h_m v(x+\delta_m)$, where each δ_m is a vector relating x to one of its neighbours. See the next subsections for two examples.

Let us try a vector $\exp(ik\cdot x) = \exp(i(k_1x_1+\cdots+k_dx_d))$. The product by H reproduces the same vector times the scalar function $h(k) = \sum_m h_m \exp(ik\cdot\delta_m)$ which are therefore the eigenvalues of H, for various real nonequivalent vectors k (Brillouin zone [30, §4]), i.e., such that each $k\cdot\delta_m \in [0,2\pi)$ or $[-\pi,\pi)$. In mathematician's lingo, $h(k)$ is the symbol of the Toeplitz matrix H (Grenander & Szegő [33, chap. 5,6, and notes of chap. 5])!

Assuming the eigenvalues to be distributed like the $k-$vectors (recall the simple $1D$ case where each k such that $\sin(kN\ell)=0$ produces an eigenvalue), the number of eigenvalues less than some E is N times the volume $\mathcal{N}(E)$ in the Brillouin zone of the $k-$vectors such that $h(k)\leqslant E$, and the Green function of the (global) density of states is trace$((x\boldsymbol{I}-\boldsymbol{H})^{-1} = \sum \dfrac{1}{x-\lambda_m} = N\displaystyle\int_{\lambda=h(k)=t}\dfrac{d\mathcal{N}(t)}{x-t} = N\int_{k\in B}\dfrac{|dk|}{x-h(k)}$.

So, there is no need to estimate numerically the density of states of a pure crystal, as the job has been done long ago. But recurrence coefficients found in this ideal case may be useful in later investigations of realistic models of true physical systems.

7. Two famous 2-dimensional lattices.

7.1. The square lattice.

The four vectors relating a site to its neighbours are $(\pm\ell,0),(0,\pm\ell)$, see fig. 1, so that $h(k_1,k_2) = 2\cos(k_1\ell)+2\cos(k_2\ell)$ (multiplied by the relevant physical energy constant, and we also ignore the multiplications by 2 and ℓ).

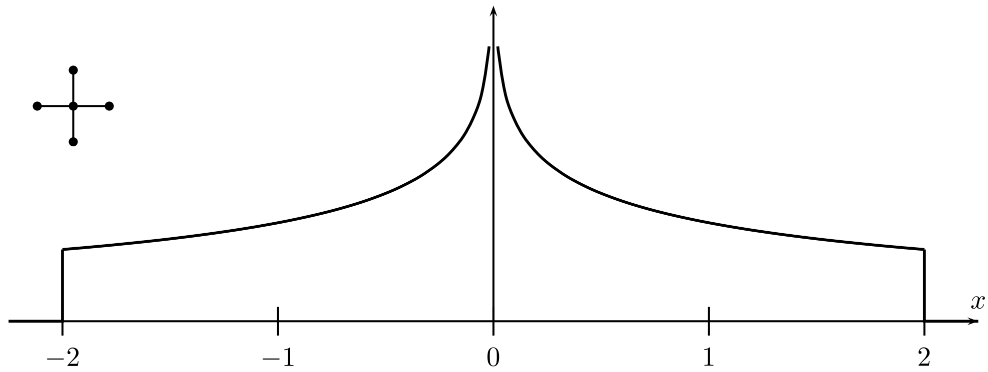

FIGURE 1. Square lattice: nearest neighbours and density of states.

Then (Economou [19, §5.3.2]),

$$S(x) = G_{0,0}(x) = (\pi)^{-2}\int_0^\pi\int_0^\pi \frac{dk_1\,dk_2}{x-\cos k_1-\cos k_2} = \frac{2}{\pi x}\boldsymbol{K}(2x^{-1}), \tag{30}$$

where $\boldsymbol{K}(u) = \displaystyle\int_0^{\pi/2}\frac{d\theta}{\sqrt{1-u^2\sin^2\theta}} = \int_0^1\frac{dr}{\sqrt{(1-r^2)(1-u^2r^2)}}$ is the complete elliptic integral of the first kind of modulus u (the $(\pi)^{-2}$ factor is for convenience).

Indeed, we integrate in k_2 for a given k_1, seeing that the integral from 0 to π is the half of the integral on the circle of $\dfrac{d\zeta/(i\zeta)}{x-\cos k_1-(\zeta+1/\zeta)/2}$, where $\zeta=\exp(ik_2)$, so π times the residue of

$-2/[\zeta^2-2(x-\cos k_1)\zeta+1]$ at the pole in the unit disk, and this residue is $\dfrac{1}{\sqrt{(x-\cos k_1)^2-1}}$, and $\dfrac{dk_1}{\sqrt{(x-\cos k_1)^2-1}} = \dfrac{\sqrt{1-\alpha^2}\,d\xi}{\sqrt{(1-\xi^2)[x+1-\alpha+((x+1)\alpha-1)\xi][x-1-\alpha+((x-1)\alpha-1)\xi]}}$ if $\cos k_1 = \dfrac{\xi+\alpha}{1+\alpha\xi}$. If α is such that $\dfrac{(x+1)\alpha-1}{x+1-\alpha} = -\dfrac{(x-1)\alpha-1}{x-1-\alpha}$, we find $\dfrac{dk_1}{\sqrt{(x-\cos k_1)^2-1}} = \dfrac{\alpha\,d\xi}{\sqrt{(1-\xi^2)(1-\alpha^4\xi^2)}}$ when $\alpha+\alpha^{-1}=x$, so the result is $2\alpha\pi^{-1}\boldsymbol{K}(\alpha^2) = \dfrac{2\alpha}{\pi(1+\alpha^2)}\boldsymbol{K}\left(\dfrac{2\alpha}{1+\alpha^2}\right)$, from the Gauss-Landen transformation formula (Jahnke & Emde [41, chap. V, §2.2], NIST [60, §19.8]), whence the result (30).

1	1.000000000				
2	1.118033989	0.1203081542			
3	0.9746794345	-0.1292279653			
4	1.037456404	0.1643807059			
5	0.9839628997	-0.1692895338			
6	1.020931612	0.1876981566			
7	0.9885010320	-0.1913801051			
8	1.014170249	0.2032383673			
9	0.9911165775	-0.2061868767			
10	1.010573403	0.2146792890			
16	1.005830221	0.2369760223	0.3381889872	(-0.2806219250)	0.3954242842
32	1.002516216	0.2655192494	0.3796921578	(-0.3956931479)	0.4419469138
64	1.001117839	0.2894108176	0.4088686585	(-0.4968111936)	0.4672216597
128	1.000505800	0.3093937275	0.4292911869	(-0.5817461016)	0.4803475080
256	1.000231686	0.3261864584	0.4437355750	(-0.6518307097)	0.4870687392
512	1.000107052	0.3404045226	0.4541490357	(-0.7095751974)	0.4905961484
1024	1.000049789	0.3525479246	0.4618385431	(-0.7575448404)	0.4925965724
2048	1.000023277	0.3630130761	0.4676645905	(-0.7979279240)	0.4938818040
4096	1.000010930	0.3721112300	0.4721909234	(-0.8324394877)	0.4948225878
8192	1.000005151	0.3800864351	0.4757888967	(-0.8623665884)	0.4955777499
16384	1.000002435	0.3871307257	0.4787065033	(-0.8886568890)	0.4962121432
32768	1.000001155	0.3933961897	0.4811126848	(-0.9120066192)	0.4967528640

TABLE 4. Square lattice: values of a_n, $n\log n[a_n-1-1/(8n^2)]$, limit after 1st degree extrapolation, slope, and limit through 2nd degree extrapolation.

The power moments are the coefficients of the expansion of $S(x) = \mu_0/x + \mu_1/x^2 + \cdots$. From the known expansion of $\boldsymbol{K}$ [60, §19.5.1] etc., $\mu_{2n+1}=0, \mu_{2n} = \left(\dfrac{1\times 3\times\cdots(2n-1)}{n!}\right)^2 = \dfrac{1}{\pi}\left(2^n\dfrac{\Gamma(n+1/2)}{\Gamma(n+1)}\right)^2 = 1, 1, 9/4, 25/4, 1225/64, \ldots$

As the spectrum is $[-2,2]$ (the extreme values of $\cos k_1+\cos k_2$), the Chebyshev moments are here the moments of $T_n(x/2) = 1, x/2, (x^2-2)/2, (x^3-3x)/2, (x^4-4x^2+2)/2, \ldots$, so $\nu_0=1, \nu_2=-1/2, \nu_4=1/8, \nu_6=-1/8, \ldots$ which must of course be computed in a sensible way, as they seem fortunately to be much smaller than the μ_ns. We need an expansion of $S(x)$ in negative powers of $z = x/2+\sqrt{x^2/4-1}$, from (27). By a stroke of luck, $z=1/\alpha$ used in the proof of (30), so we return to an intermediate result $S(x) = 2/(\pi z)\boldsymbol{K}(z^{-2})$ and apply (27) $\nu_0+\displaystyle\sum_1^\infty \frac{2\nu_n}{z^n} = \frac{2(z-z^{-1})}{\pi z}\boldsymbol{K}(z^{-2})$, whence $\nu_0=1, \nu_2=-1/2$, and $\nu_{4n} = -\nu_{4n+2} = \dfrac{1}{2^{2n+1}}\left(\dfrac{1\times 3\times\cdots(2n-1)}{n!}\right)^2, n=1,2,\ldots$

It is then possible to compute tens of thousands recurrence coefficients with the algorithm of § 3.2. Some of them are given in Table 4. As $\theta_c = \pi/2$, we expect $a_n - a_\infty \approx f_n \cos(n\pi + \varphi_c) = (-1)^n f_n \cos\varphi_c$. There is also a $1/(8n^2)$ Legendre-Jacobi contribution from the endpoints. After subtraction of this $1/(8n^2)$, the $(-1)^n$ behaviour is clear on the 10 first items of the table. The amplitude f_n of (14) being thought to decrease like $1/(n \log n)$ from conjecture 4.4, we consider $\rho_n = n \log n(a_n - 1 - 1/(8n^2))$, the limit is reached so slowly that values of ρ_n are shown on powers of 2. Assuming a $A + B/\log n$ behaviour, the slope B is estimated from two successive values, and the limit A by $\rho_n - B/\log n$ (Neville extrapolation). With $\{a, b, c\} = \{-2, 2, 0\}$, the conjecture 4.4 expects the limit 1/2. A second degree extrapolation makes this guess even more credible.

The graph of the weight function in Fig. 1 is established from $\mp\pi w(x) =$ imaginary part of the limit of $S(x \pm \varepsilon i)$ (Sokhotskyi-Plemelj [39, §14.1]) for x in the spectrum. $S(x)$ is computed as $\dfrac{1}{x - b_0 - \dfrac{a_1^2}{x - b_1 - \ddots}}$ which diverges on the spectrum. This problem is solved by replacing $\dfrac{a_N^2}{x - b_N - \dfrac{a_{N+1}^2}{\ddots}}$ by $\dfrac{a_\infty^2}{x - b_\infty - \dfrac{a_\infty^2}{\ddots}} = a_\infty/z = [x - b_\infty - \sqrt{(x-a)(x-b)}]/2$ which has a well-definite imaginary part on the two sides of the spectrum $[a, b]$. This is the termination method of Haydock & Nex [37], and Lorentzen, Thron, and Waadeland [15,47,68] going back to Wynn [76,77]. Máté, Nevai, and Totik [53,58] introduced the use of Turán determinants $p_n^2(x) - p_{n-1}(x)p_{n+1}(x)$ as a way to recover the weight function when n is large. Indeed, when (17a) applies,

$$\begin{bmatrix} p_n(x) & p_{n+1}(x) \\ p_{n-1}(x) & p_n(x) \end{bmatrix} \approx \frac{1}{\sqrt{2\pi}} \begin{bmatrix} -1 & 1 \\ -z^{-1} & z \end{bmatrix} \begin{bmatrix} z^n \exp(\lambda(z^{-1})) & 0 \\ 0 & z^{-n}\exp(\lambda(z)) \end{bmatrix} \begin{bmatrix} -1 & -z \\ 1 & z^{-1} \end{bmatrix},$$

so that the determinant $\approx -(2\pi)^{-1}(z - z^{-1})^2 \exp(\lambda(z^{-1}) + \lambda(z)) = (2a_\infty^2\pi)^{-1}\sqrt{(x-a)(b-x)}/w(x)$. The termination formula, and the Turán determinants formula are extended to spectra of several intervals = formulas for limit $p-$periodic continued fractions with $p > 1$ [15, 47, 71].

Of course, the formula (30) is considered too.

7.2. **Hexagonal lattice: *graphene*.**

One half of the sites (the "A" sites) of the hexagonal arrangement of fig. 2 are related to their neighbours through the three vectors $(1/2 \pm \sqrt{3}/2), (-1, 0)$, and these neighbours make the other half (the "B" sites) with $(-1/2 \pm \sqrt{3}/2), (1, 0)$ Horiguchi [40, §3], Katsnelson [42, §1.2], $h_{A\to B}(k_1, k_2) = 2e^{ik_1/2}\cos(k_2\sqrt{3}/2) + e^{-ik_1}, h_{B\to A}(k_1, k_2) = 2e^{-ik_1/2}\cos(k_2\sqrt{3}/2) + e^{ik_1}$.

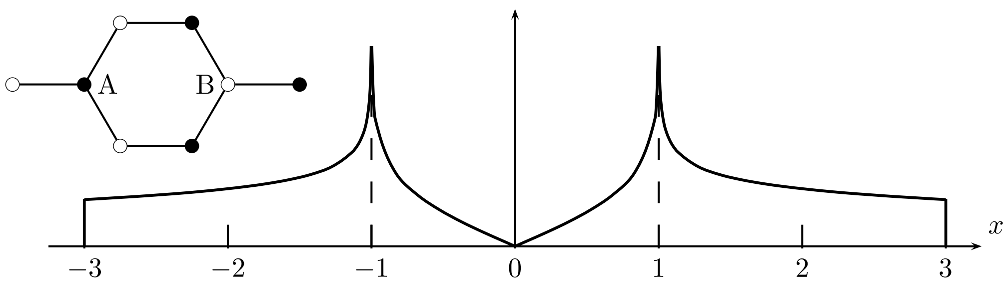

FIGURE 2. Graphene: nearest neighbors and density of states.

Using a matrix symbol for a short while, we see that the Hamiltonian operator acts on a vector $\exp(ik\cdot x)$ where the $A-$sites and the $B-$sites are considered separately, as $\begin{bmatrix} 0 & h_{A\to B}(k) \\ h_{B\to A}(k) & 0 \end{bmatrix}$, so that the eigenvalues are $E(\xi) = \pm\sqrt{h_{A\to B}(k)h_{B\to A}(k)} = \pm\sqrt{4\cos^2\xi_2 + 4\cos\xi_1\cos\xi_2 + 1}$, where $\xi_1 = 3k_1/2, \xi_2 = k_2\sqrt{3}/2)$, and the relevant Green function is

$$\begin{aligned} S(x) = G_{0,0}(x) &= \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \left[\frac{1}{x-E(\xi)} + \frac{1}{x+E(\xi)}\right] d\xi_1 d\xi_2 \\ &= \frac{x}{\pi^2}\int_0^\pi\int_0^\pi \frac{d\xi_1 d\xi_2}{x^2 - 4\cos^2\xi_2 - 4\cos\xi_1\cos\xi_2 - 1} \\ &= \frac{\sqrt{ux}}{\pi}\boldsymbol{K}(u), \text{ where } u = \frac{x^4-6x^2-3-\sqrt{(x^2-1)^3(x^2-9)}}{8x}. \end{aligned} \tag{31}$$

The last formula [40] is established by a first integral in $\xi_1 = -i\log\zeta$ so that we integrate $-id\zeta/[(x^2-4\cos^2\xi_2-1)\zeta - 2(\zeta^2+1)\cos\xi_2]$ on the unit circle, and we integrate the residue on ξ_2 as $\dfrac{x}{\pi}\displaystyle\int_0^\pi \frac{d\xi_2}{\sqrt{(x^2-1-4\cos^2\xi_2)^2 - 16\cos^2\xi_2}} = \frac{2x}{\pi}\int_0^{\pi/2}\frac{d\xi_2}{\sqrt{x^4-6x^2+1-4(x^2-1)\cos(2\xi_2)+4\cos^2(2\xi)}}$ $= \dfrac{x}{\pi}\displaystyle\int_{-1}^1 \frac{d\cos(2\xi_2)}{\sqrt{[1-\cos^2(2\xi_2)][x^4-6x^2+1-4(x^2-1)\cos(2\xi_2)+4\cos^2(2\xi_2)]}}$. As before, we change the variable $\cos(2\xi_2) = \dfrac{\eta+\alpha}{1+\alpha\eta}$, resulting in $\dfrac{x}{\pi}\displaystyle\int_{-1}^1 \frac{\sqrt{1-\alpha^2}\,d\eta}{\sqrt{[1-\eta^2][(x^4-6x^2+1)(1+\alpha\eta)^2 - 4(x^2-1)(1+\alpha\eta)(\eta+\alpha) + 4(\eta+\alpha)^2)]}}$. We keep only even powers of η if $\alpha+\alpha^{-1} = (x^2-5)/2$, and we have then $\dfrac{\alpha x}{\pi\sqrt{1+2\alpha}}\displaystyle\int_{-1}^1\frac{d\eta}{\sqrt{[1-\eta^2][1-u^2\eta^2)]}}$, with $u^2 = \alpha^3\dfrac{2+\alpha}{1+2\alpha} = \left(\dfrac{\alpha(2+\alpha)}{x}\right)^2 = \left(\dfrac{\alpha^2 x}{1+2\alpha}\right)^2$. Note that $\alpha = (\sqrt{x^2-1}-\sqrt{x^2-9})^2/8 \sim 2/x^2$ and $u = (\alpha+2\alpha^2)/x = [x^4-6x^2-3-\sqrt{(x^2-1)^3(x^2-9)}]/(8x) = 8x/[x^4-6x^2-3+\sqrt{(x^2-1)^3(x^2-9)}] \sim 4/x^3$ when x is large.

The properties of the density of states in fig. 2 follow from the last line of (31) as we follow the imaginary part of $S(x-i\varepsilon)$: u is nonreal when $x \in (1,3)$ and $(-3,-1)$. For x between -1 and 1, u is real but outside $(-1,1)$, see table 5. Near $x=1$, $u = -1 + i(x-1)^{3/2} + \cdots$, $\boldsymbol{K}(u) \sim \log(4/\sqrt{1-u^2}) \sim (-3/4)\log|x-1| +$ const., [1, 17.3.26] [41, chap. V, §C.1 and 3], $S(x) \sim -(3i)/(4\pi)\log|x-1| +$ const. Near $x=3$, the limit imaginary part of $\boldsymbol{K}$ is $\pi/4$, so $\sqrt{3}/4 = 0.433013...$ for S. Near $x=0$, $u \sim -3/(4x)$, $\boldsymbol{K}(u) \sim \pi/(2u)$ (from the Gauss-Landen formula seen above), and $\mathrm{Im}(S(x)) \sim |x|/\sqrt{3}$. The complete elliptic integral $\boldsymbol{K}$ is computed in table 5 by the AGM method [1, 6, 60].

Check of first power moments: μ_n is the constant Fourier coefficient of the power $(4\cos^2\xi_2 + 4\cos\xi_1\cos\xi_2+1)^n$, $S(x) = \dfrac{1}{x}+\dfrac{3}{x^3}+\dfrac{15}{x^5}+\dfrac{93}{x^7}+\dfrac{639}{x^9}+\ldots = \dfrac{1|}{|x} - \dfrac{3|}{|x} - \dfrac{2|}{|x} - \dfrac{3|}{|x} - \dfrac{5/3|}{|x} - \dfrac{44/15|}{|x} - \dfrac{393/220|}{|x} - \cdots$ The Chebyshev moments are the moments of $T_n(x/3) = 1, x/3, 2x^2/9-1, 4x^3/27-x, 8x^4/81-8x^2/9+1, \ldots$ as the spectrum is $[-3,3]$ (extreme real values of $\pm$ the square root of $4\cos^2\xi_2 + 4\cos\xi_1\cos\xi_2 + 1 = (\cos\xi_1 + 2\cos\xi_2)^2 + \sin^2\xi_1$), so $\nu_0 = 1, \nu_2 = -1/3, \nu_4 = -5/27, \ldots$ More instances are $\nu_6 = 47/243, \nu_8 = -167/729, \nu_{10} = 1013/6561$.

x	u	S(x)
10.000 - 0.01i	0.004257 + 0.00001332i	0.103160 + 0.000109821i
5.000 - 0.01i	0.042448 + 0.00031193i	0.230453 + 0.000617812i
3.200 - 0.01i	0.356839 + 0.00913118i	0.552670 + 0.00722059i
3.100 - 0.01i	0.481506 + 0.0174922i	0.651771 + 0.0142386i
3.000 - 0.01i	0.838022 + 0.138058i	0.976877 + 0.217790i
2.900 - 0.01i	0.716970 + 0.644469i	0.666148 + 0.427229i
...		
2.000 - 0.01i	-0.679582 + 0.717773i	0.367256 + 0.532098i
...		
1.200 - 0.01i	-0.990512 + 0.0830288i	0.264783 + 0.793926i
1.100 - 0.01i	-0.995069 + 0.0302862i	0.242050 + 0.927258i
1.000 - 0.01i	-1.00071 + 0.000704934i	0.382753 + 1.42850i
0.900 - 0.01i	-1.03330 - 0.00524755i	-0.446485 + 0.830781i
0.800 - 0.01i	-1.10216 - 0.00857685i	-0.431632 + 0.629673i
...		
0.200 - 0.01i	-3.77435 - 0.185309i	-0.195181 + 0.123569i
0.100 - 0.01i	-7.44245 - 0.740894i	-0.119693 + 0.0668312i
- 0.01i	- 74.9983i	0.0209638i
-0.100 - 0.01i	7.44245 - 0.740894i	0.119693 + 0.0668312i

TABLE 5. Graphene: values of x, u, and the Stieltjes, or Green, function $S(x)$ near the spectrum $[-3, 3]$.

From (27), $\nu_0/2$ and $\nu_n, n > 0, =$ the coefficients of z^{-n} of $\dfrac{3(z-z^{-1})}{4} S\left(x = \dfrac{3(z+z^{-1})}{2}\right) =$ $\dfrac{3(z-z^{-1})}{4}\left[\dfrac{2}{3(z+z^{-1})} + 3\left(\dfrac{2}{3(z+z^{-1})}\right)^3 + \cdots\right] = \dfrac{1}{2} - \dfrac{1}{3z} + \cdots$

How to compute accurately a very large set of these coefficients? A recurrence relation is an invaluable tool for efficient and economical computation of a sequence. Of course, one must be lucky, or clever, enough to find such a relation. For instance, Piessens & *al.* [61,62] find recurrence relations for examples of Chebyshev modified moments.

An important family of recurrence relations is found for sequences of Taylor (or Laurent, or Frobenius) coefficients of solutions of linear differential equations with rational coefficients (Laplace method, see Milne-Thomson [56, chap. 15], Bender & Orszag [5, § 3.2, 3.3]). Let $F(x) = \sum_0^\infty c_n x^n$ be a solution of the differential equation $\sum_{m=0}^{\delta} X_m(x) d^m F(x)/dx^m = \sum_0^\infty \alpha_n x^n$, where $X_m(x)$ is the polynomial $\sum_{p=0}^{d} \chi_{m,p} x^p$, and where the right-hand side is a known expansion. Then, substituting the unknown expansion $\sum c_r x^r$ of $F(x)$ into the differential equation, $\sum_{m=0}^{\delta} X_m(x)[\sum_{r=m}^{\infty} r(r-1)\cdots(r-m+1)c_r x^{r-m}] = \sum_0^\infty \alpha_n x^n$, and we gather the terms contributing to the x^n power:
$\sum_{m=0}^{\delta}\sum_{p=0}^{d} \chi_{m,p}(n+m-p)(n+m-p-1)\cdots(n-p-1)c_{n+m-p} = \alpha_n$, $n = 0, 1, \ldots$, which is the sought recurrence relation involving $c_{n+\delta}, \ldots, c_{n-d}$.

We apply this programme to the coefficients of the expansion

$$3(z-z^{-1})S(x)/4 = 3(z-z^{-1})\sqrt{ux}\boldsymbol{K}(u)/(4\pi) = \frac{\nu_0}{2} + \sum_{n=1}^{\infty} \frac{\nu_{2n}}{z^{2n}} \tag{32}$$

where u is the algebraic function $\dfrac{x^4 - 6x^2 - 3 - \sqrt{(x^2-1)^3(x^2-9))}}{8x}$, and where $x = 3(z+1/z)/2$.

First, $u(1-u^2)d^2\boldsymbol{K}/du^2+(1-3u^2)d\boldsymbol{K}/du-u\boldsymbol{K}=0$ [60, § 19.4.8] turns into the more beautiful $\dfrac{d^2(\sqrt{u}\,\boldsymbol{K})}{du^2}-2\dfrac{u}{1-u^2}\dfrac{d(\sqrt{u}\,\boldsymbol{K})}{du}+\dfrac{\sqrt{u}\,\boldsymbol{K}}{4u^2}=0.$

Next, u is the root of $u+1/u=(x^4-6x^2-3)/(4x)$ behaving as $4/x^3$ for large x, we translate in z from $x=3(z+1/z)/2$, leading to the rather formidable

$$u,\frac{1}{u}=\frac{27z^4+36z^2+2+36z^{-2}+27z^{-4}\mp(z-z^{-1})(9z^2+14+9z^{-2})^{3/2}}{64(z+z^{-1})} \tag{33}$$

So, we differentiate $u+u^{-1}=\dfrac{27z^4+36z^2+2+36z^{-2}+27z^{-4}}{32(z+z^{-1})}$ as

$(1-u^{-2})du=\dfrac{81z^5+171z^3+106z-106z^{-1}-171z^{-3}-81z^{-5}}{32z(z+z^{-1})^2}dz$, or

$$\frac{du}{u\,dz}=\frac{(z^2-1)(9z^2+14+9/z^2)^2}{32(z^2+1)^2(u-u^{-1})}=-\frac{(9z^2+14+9/z^2)^{1/2}}{z^2+1}, \tag{34}$$

which is already better looking than before, and we build the differential equation for $\sqrt{u}\,\boldsymbol{K}$ in the slightly modified form $u\dfrac{d}{du}\left[u\dfrac{d\,\sqrt{u}\boldsymbol{K}(u)}{du}\right]-\dfrac{u+u^{-1}}{u-u^{-1}}u\dfrac{d\,\sqrt{u}\boldsymbol{K}(u)}{du}+\dfrac{\sqrt{u}\boldsymbol{K}(u)}{4}=0$ with respect to the variable z:

$$\frac{z^2+1}{(9z^2+14+9/z^2)^{1/2}}\frac{d}{dz}\left[\frac{z^2+1}{(9z^2+14+9/z^2)^{1/2}}\frac{d\sqrt{u}\,\boldsymbol{K}}{dz}\right] \\ +\frac{27z^4+36z^2+2+36z^{-2}+27z^{-4}}{(z-z^{-1})(9z^2+14+9/z^2)^{3/2}}\frac{z^2+1}{(9z^2+14+9/z^2)^{1/2}}\frac{d\sqrt{u}\,\boldsymbol{K}}{dz}+\frac{\sqrt{u}\,\boldsymbol{K}}{4}=0.$$

Finally, we turn to the full function of (27) and (31), say $F(z)=(z-z^{-1})S(x)=$ constant times $(z-z^{-1})\sqrt{ux}\boldsymbol{K}(u)$ by substituting $\sqrt{u}\,\boldsymbol{K}(u)$ into const. $(z-z^{-1})^{-1}(z+z^{-1})^{-1/2}S$

$$\frac{z^2+1}{(9z^2+14+9/z^2)^{1/2}}\frac{d}{dz}\left[\frac{z^2+1}{(9z^2+14+9/z^2)^{1/2}}\frac{d(z-z^{-1})^{-1}(z+z^{-1})^{-1/2}F}{dz}\right] \\ +\frac{(z^2+1)(27z^4+36z^2+2+36z^{-2}+27z^{-4})}{(z-z^{-1})(9z^2+14+9/z^2)^2}\frac{d(z-z^{-1})^{-1}(z+z^{-1})^{-1/2}F}{dz} \\ +\frac{(z-z^{-1})^{-1}(z+z^{-1})^{-1/2}F}{4}=0,\ \text{so}$$

$$(z^2+1)^2(9z^2+14+9z^{-2})(z-z^{-1})^2d^2F/dz^2+(z^2+1)(9z^4-14z^2-72-42z^{-2}-9z^{-4})(z-z^{-1})dF/dz \\ +8(3z^4+18z^2+22+18z^{-2}+3z^{-4})F=0$$

Now, put $Fz=\nu_0/2+\sum_1^\infty\dfrac{\nu_{2n}}{z^{2n}}$ in the differential equation $(9z^8+14z^6-9z^4-28z^2-9+14z^{-2}+9z^{-4})\sum 2n(2n+1)\nu_{2n}z^{-2n-2}-(9z^7-14z^5-81z^3-28z+63z^{-1}+42z^{-3}+9z^{-5})\sum 2n\nu_{2n}z^{-2n-1}+8(3z^4+18z^2+22+18z^{-2}+3z^{-4})[\nu_0/2+\sum\nu_{2n}z^{-2n}]=0$, and consider the contributions to z^{-2n}

$$9(n+3)^2\nu_{2n+6}+2(7n^2+35n+45)\nu_{2n+4}-9(n^2-2n-7)\nu_{2n+2}-4(7n^2-11)\nu_{2n} \\ -9(n^2+2n-7)\nu_{2n-2}+2(7n^2-35n+45)\nu_{2n-4}+9(n-3)^2\nu_{2n-6}=0, n=0,1,\dots \tag{35}$$

starting at $n=-2$ with $\nu_0 = 1/2$ (which is actually $\nu_0/2$) and $\nu_n = 0$ for $n < 0$ (the $\nu_0/2$ anomaly can be relieved if we define $\nu_{-n} = \nu_n$, remark indeed that the coefficient of ν_{2n+k} is the coefficient of ν_{2n-k} with $n \to -n$). The next items are $-1/3, -5/27, 47/243, -167/729, 1013/6561, -15653/177147, \dots$ as already seen before, but the recurrence relation (35) allows now to compute incredibly easily any number of these coefficients, one could get one million of them if needed!

The main asymptotic behaviour of ν_n follows from $S(x) \sim -(3i)/(4\pi)\log|x-1| +$ const. near $x = \pm 1$, seen above, so, near $z = \pm z_0^{\pm 1} = \pm\exp(\pm i\theta_0)$, where $\cos\theta_0 = 1/3$, $z_0 = (1+2i\sqrt{2})/3$, from (27): $(6/8)(z-1/z)S(x) \sim \pm(3\sqrt{2}/4\pi)\log(z \pm z_0^{\pm 1})$ whence $\nu_n = 0$ when n is odd, $\nu_n \sim 2\dfrac{3\sqrt{2}}{4\pi}\dfrac{z_0^n + z_0^{-n}}{n} = \dfrac{3\sqrt{2}\cos(n\theta_0)}{\pi n}$ when n is even. For instance, $\nu_{1000000} = -0.2197681875531559\ 10^{-6}$ and $(3\sqrt{2}/\pi)\cos(10^6\theta_0) = -0.2197654658865520$.

Do we really need the recursion method?? The plain Chebyshev, or Fourier, coefficients are already so efficient that they can be preferred, as discussed by Weisse & al. [73, §V.B.2, Table II]. See also Prevost [63] on weight reconstruction with Chebyshev moments.

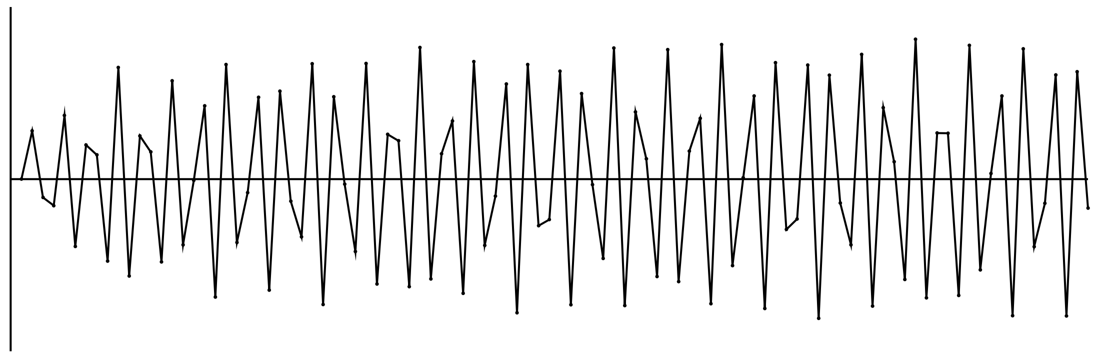

FIGURE 3. Graphene: 100 first $\rho_n = n\log n[a_n - 3/2 + (3/4)(-1)^n/n - (3/16)/n^2]$.

Anyhow, computing recurrence coefficients from modified moments yields the main behaviour $a_n \to a_\infty = (b-a)/4 = 1.5$ as expected from (8). The next correction is given by the $|x|^\alpha$ behaviour near $x=0$, with $\alpha = 1$, and is $a_n \sim a_\infty - ((b-a)\cos(n\pi)|\alpha|)/(8n) = 1.5 - 0.75(-1)^n/n$. The Jacobi-Legendre effect of the endpoints ± 3 is $(b-a)/(32n^2) = 3/(16n^2)$. The remaining behaviour times $n\log n$ believed to be the right factor $\rho_n = n\log n[a_n - 1.5 + 0.75(-1)^n/n - 0.1875/n^2]$ is shown in table 6, and is expected to behave like const. times $\cos(2n\theta_c + \varphi_c)$. Starting with a large index (here, 135), only crest values are retained, i.e., such that $2n\theta_c + \varphi_c$ happens to be very close to an integer multiple of π. The neighbouring values ρ_{n-1} and ρ_{n+1} are then very close together, that's how the interesting values of n are selected. Moreover, the almost common value of ρ_{n-1}/ρ_n and ρ_{n+1}/ρ_n must then be almost $\cos(2\theta_c) = -7/9 = -0.7777\dots$, checked in the last column of table 6 (the first approximated crest is at $n = 10$, see also Fig. 3), whereas φ/π is estimated through the fractional part of $2n\theta_c/\pi$ for these very particular values of n, of which only those in approximate geometric progression have been selected, in the hope to have a better view of the limit of $|\rho_n|$. Although the phase φ is very stable, the evolution of $|\rho_n|$ towards its limit is again excruciatingly slow. An approximate law $A + B/\log n$ is again assumed with the slope B estimated from two successive values, and A as $|\rho_n| - B/\log n$ (extrapolated value). With two contributions at ± 1 in the spectrum $[-3, 3]$, the formula from 4.4 amounts to expecting $\sqrt{2} = 1.414\dots$ which is neither close nor far from the numerical estimate $1.405\dots$

The first 69999 recurrence coefficients $a_1 - -a_{69999}$ are given in the file
`http://perso.uclouvain.be/alphonse.magnus/graphene69999.txt`
of size about 2M, with a precision of 25 digits, in the following format:

```
1.7320508075688772935274463,
1.4142135623730950488016887,
1.7320508075688772935274463,
1.2909944487358056283930885,
1.7126976771553505360155865,
...
1.4999899549568860858094207,
1.5000093070617496121273346,
```

n	an	rhon	slope	extrap.	phi/pi	rho(n-1)/rhon
1	1.732050807568877	0				
2	1.414213562373095	0.33595				
3	1.732050807568877	-0.12782				
4	1.290994448735806	-0.18423				
5	1.712697677155351	0.44419				
6	1.336549152243806	-0.46936				
7	1.628436152438179	0.23792				
8	1.419330149577324	0.16886				
9	1.556750628851699	-0.57145				
10	1.460678158360451	0.77835				
11	1.544107839921112	-0.67587				
12	1.448901939699682	0.30117				
13	1.564500085917823	0.19001				
14	1.431783794658055	-0.57642				
15	1.567701045607340	0.68518				
135	1.507049663059332	0.98260	,(0)	0.98260	0.7932	-0.7722
1383	1.500654249446685	1.11873	,(-2.07548)	1.40571	0.7922	-0.7751
2007	1.500299317783996	-1.13581	,(-2.11734)	1.41425	0.7918	-0.7767
4087	1.500149457578103	-1.15763	,(-2.09351)	1.40939	0.7902	-0.7795
8210	1.499924544322330	1.17608	,(-2.08240)	1.40713	0.7920	-0.7760
16077	1.500038998496210	-1.19159	,(-2.07718)	1.40606	0.7910	-0.7780
34062	1.499974587460581	-1.20647	,(-2.07210)	1.40503	0.7920	-0.7757
61370	1.499985980208882	-1.21710	,(-2.07231)	1.40507	0.7910	-0.7778

TABLE 6. Graphene: values of $n, a_n, \rho_n = n\log n[a_n - 3/2 + (3/4)(-1)^n/n - (3/16)/n^2]$, (slope), extrap., $\varphi/\pi, \rho_{n-1}/\rho_n$

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