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

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 two conjectures. 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).

Keywords: Numerical analysis, Integration formulas, Logarithmic singularities, Solid-state physics, 2-dimensional lattices, Graphene.

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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

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

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

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

with $P_1(x) = x - b_0$. See, among numerous other sources, Chihara's book [17], Gautschi's ones [35, 37], chap. 18 of NIST handbook [78], and other surveys [40, 61, 62].

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 $x_1, \ldots, x_N$. 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, say, $f(t) = t^N$, see that $f - p$ vanishes at $x_1, \ldots, x_N$ and will be orthogonal to all polynomials of degree $< N$ if it is a constant times P_N, so if $x_1, \ldots, x_N$ 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 [21, § 2.7], Boyd [11, chap. 4] for this discussion.

Approximate integration formulas are not only used in the 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 [11, chap. 3, 4], Fornberg [28, § 4.7], Mansell & al. [67], Shizgal [86].

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 [48, chap. 12]. For measures on the whole real line, one should use the name "Hamburger transform". P. Henrici [49, §14.6] speaks of "Cauchy integrals on straight line segments", Van Assche [90] calls S "Stieltjes transform" for (3) in all cases. "Markov function" is also used [4, 40] when it is clear that there is no danger of confusion with random processes.

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 [5, 6] $Q_n(x) = \displaystyle\int_a^b \frac{P_n(t)\, d\mu(t)}{x-t}$. 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 $\dfrac{Q_n(x)}{Q_{n-1}(x)} = \dfrac{a_n^2}{x - b_n - \dfrac{Q_{n+1}(x)}{Q_n(x)}}$, [38, 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 $x \notin [a,b]$ [49, 94].

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 [78, §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 [18] 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 [17, 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 [35], which will be considered in next section.

In some serendipitous cases, as seen in Table 1, closed-form formulas have been found [17, chapters 5 and 6] [78, § 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 $1/4, 13/28, 8795/18116, \dots$ [71].

2.2. **Asymptotic behaviour of recurrence coefficients.**

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 [61, §3.2], P. Nevai [74, §4.5], [75], and Van Assche's book [90, §2.6] for accurate statements and story.

A closer look to the Jacobi recurrence coefficients (7), Table 1 gives

$$a_n = \frac{1}{4} - \frac{(q-1)^2 + (p-q)^2 - 1/2}{16n^2} + o(n^{-2}),$$
$$b_n = \frac{1}{2} + \frac{(q-1)^2 - (p-q)^2}{8n^2} + o(n^{-2}).$$

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

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

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

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 [56, Appendix] made interesting numerical tests on problems of solid-state physics by reducing the oscillating terms through sums and products, their formulas[2] are:
$a_1 \cdots a_n = \text{constant } \times \left(\dfrac{b-a}{4}\right)^n \left(1 + \dfrac{\alpha^2+\beta^2-1/2}{4n} + o(1/n)\right)$,
$b_0 + \cdots + b_n = n\dfrac{a+b}{2} + \text{constant } + \dfrac{(b-a)(\alpha^2-\beta^2)}{8n} + o(1/n)$. The constants are known from Szegő's theory, see § 6.3. Complete expansions in powers of $1/n$ have been established when the weight function is $(b-x)^\alpha(x-a)^\beta$ times a positive analytic function on $[a,b]$ [54, Thm. 1.10], quite a strong condition. Perturbation of a Jacobi weight is considered by Nevai and Van Assche [76, § 5.2], but their trace-class condition $\sum |a_n - a_\infty| + |b_n - b_\infty| < \infty$ is rather strong too, as we will encounter expected $O(1/n)$ and $O(1/(n\log n))$ perturbations. See also L.Lefèvre et al. [58] for more applications with Jacobi polynomials.

Much more refinements will be studied in §5 and 6.

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 defined as

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

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

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

Where the left-hand side is the Gram matrix of the basis $\{R_0, \dots, R_{N-1}\}$, factored in (11) 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 [12, 13].

[2]The product $b_1 \cdots b_n$ of [56] is here $a_1^2 \cdots a_n^2$.

See also Bultheel & Van Barel [15, § 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 [41,96]), 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 [96, §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 [8].

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 [82, 83], immediately enthusiastically commented and expanded by W. Gautschi [33] whose exposition is summarized here (see also [35, § 2.1.7], [37, viii, pp. 28,36, 58–64, 92–100, 162]).

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

$$xR_k(x) = A_k R_{k+1}(x) + B_k R_k(x) + \cdots + Z_k R_{k-s}(x), \tag{12}$$

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
$\boldsymbol{v}^{(n)} = [\int_a^b P_n(t)R_0(t)d\mu(t), \int_a^b P_n(t)R_1(t)d\mu(t), \dots, \int_a^b P_n(t)R_{2N-n}(t)d\mu(t)]$, looking like the rows of the last factor of (11), for $n = 0, 1, \dots, N-1$, starting of course with the modified moments at $n = 0$. By orthogonality of P_n and polynomials of degree $< n$, one must have $\boldsymbol{v}_0^{(n)} = \boldsymbol{v}_1^{(n)} = \cdots = \boldsymbol{v}_{n-1}^{(n)} = 0$. We also define $\boldsymbol{v}^{(-1)}$ to be the null vector. Then, by (2) and (12),

$$\begin{aligned}
\boldsymbol{v}_k^{(n+1)} &= \int_a^b P_{n+1}(t)R_k(t)d\mu(t) \\
&= \int_a^b (t - b_n)P_n(t)R_k(t)d\mu(t) - a_n^2 \int_a^b P_{n-1}(t)R_k(t)d\mu(t) \\
&= \int_a^b [A_k R_{k+1}(t) + (B_k - b_n)R_k(t) + \cdots + Z_k R_{k-s}(t)]P_n(t)d\mu(t) - a_n^2 \int_a^b P_{n-1}(t)R_k(t)d\mu(t) \\
&= A_k \boldsymbol{v}_{k+1}^{(n)} + (B_k - b_n)\boldsymbol{v}_k^{(n)} + \cdots + Z_k \boldsymbol{v}_{k-s}^{(n)} - a_n^2 \boldsymbol{v}_k^{(n-1)},
\end{aligned}$$

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 $\boldsymbol{v}_n^{(n+1)} = 0 \Rightarrow b_n = B_n + [A_n \boldsymbol{v}_{n+1}^{(n)} - a_n^2 \boldsymbol{v}_n^{(n-1)}]/\boldsymbol{v}_n^{(n)} = B_n + A_n \boldsymbol{v}_{n+1}^{(n)}/\boldsymbol{v}_n^{(n)} - A_{n-1}\boldsymbol{v}_n^{(n-1)}/\boldsymbol{v}_{n-1}^{(n-1)}$.

See also that $\boldsymbol{v}_k^{(n+1)}$ needs $\boldsymbol{v}_{k+1}^{(n)}$, that's why we need the $\boldsymbol{v}_k^{(0)}$s up to $k = 2N$, in order to have a correct $\boldsymbol{v}_N^{(N)}$.

There will be much ado later on about the Chebyshev polynomials on $[a,b]: R_0(t)\equiv 1, R_1(t)= T_1((2t-a-b)/(b-a))=(2t-a-b)/(b-a), R_2(t)=T_2((2t-a-b)/(b-a))=2((2t-a-b)/(b-a))^2-1,\dots$ satisfying $tR_n(t)=(b-a)R_{n-1}(t)/4+(a+b)R_n(t)/2+(b-a)R_{n+1}(t)/4$.
Remark. If we have a software allowing fast shift vector operations shiftleft$([a_1,\dots,a_N])= [a_2,\dots,a_N,0]$, shiftright$([a_1,\dots,a_N])=[0,a_1,\dots,a_{N-1}]$, then
$\boldsymbol{v}^{(n+1)}=(b-a)[\text{shiftleft}(\boldsymbol{v}^{(n)})+\text{shiftright}(\boldsymbol{v}^{(n)})]/4+(a+b)\boldsymbol{v}^{(n)}/2-a_n^2\boldsymbol{v}^{(n-1)}-b_n\boldsymbol{v}^{(n)}$ [36].

4. 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 $\nu_n=\int_a^b R_n(t)\,w(t)\,dt$:

4.1. **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,*

$$S(x)=\sum_0^\infty \frac{\nu_n}{\|R_n\|_R^2}Q_n(x), \tag{13}$$

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

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 $w(t)/w_R(t)$
$=\sum_{n=0}^\infty [\int_a^b (w(u)/w_R(u))w_R(u)R_n(u)du=\nu_n]R_n(t)/\|R_n\|_R^2$ 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 makes 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 $\int_a^b p^2w\,dx/\int_a^b p^2w_R\,dx$, 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 [8].

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 [7], Gautschi [34].

For Legendre functions, the connection between Laurent expansions and expansions in functions of the second kind is given by the Heine's series $(x-t)^{-1} = \sum_0^\infty (2m+1)P_m(t)Q_m(x)$, $-1 < t < 1, x \notin [-1, 1]$ (NIST [78, § 14.28.2], etc.), so that, gathering the t^n terms, $\dfrac{1}{x^{n+1}} = \sum_0^n \dfrac{d^n P_m(0)/dt^n}{n!} Q_m(x)$, 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:

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

See Area *et al.* [5,6] for more identities.

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

4.2. **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*

$$Q_n(x) = \int_a^b \frac{T_n((2t-a-b)/(b-a))\, dt}{(x-t)\sqrt{(t-a)(b-t)}} = \frac{\pi}{a_\infty z^n (z - 1/z)}, \tag{14}$$

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

This formula (14) is seen as an exercise in many textbooks, as Davis & Rabinowitz [21, § 1.13], sometimes from the finite part (Hilbert transform) of (14) when $x \in (a, b)$, known to be $-(\pi/(2a_\infty))U_{n-1}(\cos\theta)$ [1, 22.13.3], [68, eq. 9.22a], also used by Weisse & al. [95, eq. (14)]. Then, when $x = b_\infty + 2a_\infty \cos\theta \pm i\varepsilon$ is close to $[a, b]$, we add $\pm\pi i T_n(\cos\theta)/\sqrt{(x-a)(b-x)}$ (Sokhotskyi-Plemelj [49, §14.1]), and (14) is restored in a neighbourhood of $[a, b]$. For a fast proof of (14) for all x, recalling that the functions of the two kinds share the same recurrence relations, so $Q_n(x)$ must be a linear combination of z^n and z^{-n}, which must remain bounded for large x, so $Q_n(x) = Q_0(x)\, z^{-n}$. Put $t = (a+b)/2 + ((b-a)/2)\cos\varphi = b_\infty + 2a_\infty \cos\varphi$, then $Q_0(x) = \displaystyle\int_0^\pi \frac{d\varphi}{x - b_\infty - 2a_\infty\cos\varphi} = \int_0^\pi \frac{2d\varphi}{a_\infty(z + z^{-1} - 2\cos\varphi} = \frac{1}{2i}\oint \frac{de^{i\varphi}}{a_\infty(z - e^{i\varphi})(e^{i\varphi} - z^{-1})} = \frac{\pi/a_\infty}{z - z^{-1}}$, as only the residue at $e^{i\varphi} = z^{-1}$ is to be considered, as $|z| > 1$.

It will also be recalled in § 6.3 that the asymptotic formula (22b) 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 (14) in [49, § 14.6, Problem 2] with the symbol "U_n" for our Q_n.

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

$$\frac{(b-a)(z-z^{-1})}{2} S\left(x = \frac{a+b}{2} + \frac{(b-a)(z+z^{-1})}{4}\right) = 2\nu_0 + \sum_1^\infty \frac{4\nu_n}{z^n}. \tag{15}$$

Indeed, put (14) in (13)

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

5. Weights with logarithmic singularities. Endpoint singularity.

5.1. **Numerical tests.**

B. Danloy [20] 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 [1,78] 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 $\int_0^x R_n(t)dt = (R_{n+1}(x) - R_{n-1}(x))/(2(2n+1))$ [28, p.157], whence the modified moments

$$\nu_0 = 1, \nu_n = -\int_0^1 R_n(t)\log t\,dt$$
$$= \int_0^1 \frac{R_{n+1}(t) - R_{n-1}(t)}{2(2n+1)t}dt = -\int_0^1 \frac{R_n(t) + R_{n-1}(t)}{2(n+1)t}dt = \frac{(-1)^n}{n(n+1)}, n = 1,2,\ldots$$

[78, 14.18.6 Christoffel Darboux], also a special case of Jacobi polynomials formulas by Gautschi [36, eq. (16)]. Powers of logarithms are considered by Sidi [87]. It is then possible to compute safely thousands of recurrence coefficients, as done in table 2.

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 $a_n = 1/4 - \dfrac{1/32}{n^2} + o(n^{-2}), b_n = \dfrac{1}{2} - \dfrac{1}{8n^2} + o(n^{-2})$, from (9) when $a = 0, b = 1$, and $\alpha = 1, \beta = 0$.

The next terms in the asymptotic description of a_n and b_n is suspected to behave like $(n\log n)^{-2}$:

5.2. **Conjecture.** *If the weight function has no interior singularity, and if $w(x)/[-(x-a)^\beta\log(x-a)]$ and $w(x)/(b-x)^\alpha$ have positive bounded limits at $x = a$ and $x = b$, then there are constants A and B such that*

$$\begin{aligned} a_n &= \frac{b-a}{4}\left(1 - \frac{\alpha^2+\beta^2-1/2}{4n^2}\right) + \frac{A}{(n\log n)^2} + o((n\log n)^{-2}), \\ b_n &= \frac{a+b}{2} - \frac{(b-a)(\alpha^2-\beta^2)}{8n^2} + \frac{B}{(n\log n)^2} + o((n\log n)^{-2}). \end{aligned} \tag{16}$$

It is also conjectured that $B = -2A$.

As logarithmic terms vary so slowly, the best way to recover them is to take a sequence of values of n such that the suspected logarithmic term follows an approximate arithmetic progression. Should we look for a first power of $\log n$, a geometric progression of n will do the trick, as will be done in table 4, as a check of the conjecture of §6.2. Here, we take $n =$ the integer part of $\exp\sqrt{Ck}$, $k = 1,2,\ldots$, and look in table 2 at $a_n, n^2(1/4 - a_n)$, expected to behave like $1/32 - A/\log^2 n$, so, $e_k := 1/[n^2(1/4-a_n) - 1/32] \sim -\log^2 n/A \sim Ck/A$, and $-1/A$ is recovered through the difference $(e_k - e_{k-1})/C$ ($C = 5$ in our example), and by the ratio $e_k/(Ck)$; for b_n, consider $f_k = 1/[1/8 - n^2(1/2 - b_n)] \sim Ck/B$.

We find here A and B close to -0.044 and 0.085. One would like to investigate further the dependence of A and B on α, β, more powers of logarithms... We have at least an interesting relation to the interior singularity conjecture of §6.2: let $x = a + (b-a)t^2$, then $P_n(x) = (b -$

5k	n	an	n^2(1/4-an)	e_k	-1/A	bn	n^2(1/2-bn)	f_k	1/B
	0					0.250000000000			
	1	0.220479275922	0.02952			0.464285714286	0.0357		
	2	0.242249473181	0.03100			0.485482446456	0.0581		
	3	0.246431702341	0.03211			0.492103081871	0.0711		
	4	0.247955681921	0.03271			0.495028498758	0.0795		
	5	0.248678124353	0.03305			0.496579511644	0.0855		
...									
45	819	0.249999952108	0.03212	1143.6	21.8	0.499999816678	0.1230	491.5	13.3
					25.4				10.9
50	1177	0.249999976866	0.03205	1253.6	22.0	0.499999911064	0.1232	557.2	13.2
					25.1				11.1
...									
95	17099	0.249999999892	0.03169	2263.7	22.5	0.499999999576	0.1241	1114.5	11.9
					23.8				11.7
100	22026	0.249999999935	0.03167	2376.4	22.5	0.499999999744	0.1241	1173.3	11.8
					23.8				11.7

TABLE 2. Recurrence coefficients values and behaviour for the logarithmic weight $-\log t$ on $(0,1)$. When n (of the form integer part of $\exp\sqrt{5k}$) is large enough, $e_k := 1/[n^2(1/4-a_n)-1/32] \sim -\log^2 n/A \sim 5k/A$ is shown, leading to estimates of $-1/A$ by two different methods; for b_n, $f_k = 1/[1/8-n^2(1/2-b_n)] \sim 5k/B$ is shown.

$a)^n\tilde P_{2n}(t)$, where $\tilde P_{2n}$ is the even monic orthogonal polynomial of degree $2n$ with respect to the even weight function $|t|w(a+(b-a)t^2)$ on $[-1,1]$, as well known ([17, chap. 1,§8], etc.), as is the recurrence relation:

$$\tilde P_{2n+2}(t) = t\left[\tilde P_{2n+1}(t) = t\tilde P_{2n}(t) - \tilde a_{2n}^2 \frac{\tilde P_{2n}(t)+\tilde a_{2n-1}^2\tilde P_{2n-2}(t)}{t}\right] - \tilde a_{2n+1}^2\tilde P_{2n}(t),$$

so, $a_n = (b-a)\tilde a_{2n}\tilde a_{2n-1}, b_n = a+(b-a)(\tilde a_{2n}^2+\tilde a_{2n+1}^2)$. As $\tilde a_n = 1/2 + (-1)^n\tilde A/(n\log n)+\cdots$ is expected from the conjecture of § 6.2 (here, $c=0$ and $\theta_c = \pi/2$ in (18)), then a part of (16) follows, with $A = -(b-a)\tilde A^2/4$. We have no check for A (just its negative sign), as $|t|\log|t|$ singularities are not considered in (21).

5.3. **Trying multiple orthogonal polynomials.**

Warning: this subsection deals with a trend which proved not to be fruitful in the present case, but could be inspiring in other situations. Fact is that I do not know any other explicit family of orthogonal (of some sort) polynomials with respect to a logarithmic weight function.

Quite another trend is given by known formulas for some multiple orthogonal polynomials, summarized here [40, § 12]: the polynomial $R_n = R_{\{n_1,\dots,n_p\}}$ of degree $n = n_1+\cdots n_p$ is a multiple orthogonal polynomial with respect to the measures $d\mu_1,\dots,d\mu_p$ if R_n is orthogonal to polynomials of degree $< n_1$ with respect to $d\mu_1$, of degree $< n_2$ w.r.t. $d\mu_2,\dots$, 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 [14]. An interesting recurrence relation (12) with $s=p$ occurs when[3] $n_j = 1+\lfloor (n-j)/p\rfloor, j = 1,\dots,p$.

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 [3]. 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 and $\alpha_2\to 0$, then the orthogonality holds with respect to the constant weight and the limit of

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

$\dfrac{x^{\alpha_2}-x^{\alpha_1}}{\alpha_2-\alpha_1}$ which is $\log x$, there we are: R_n does 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 $R_n(x) = \dfrac{1}{n_1!\,n_2!}\dfrac{d^{n_2}}{dx^{n_2}}\left[x^{n_2}\dfrac{d^{n_1}}{dx^{n_1}}x^{n_1}(x-1)^n\right]$ [3, §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

$$\begin{aligned}
xR_n(x) &= \frac{4(n+1)^2(n+2)}{(3n+2)^2(3n+4)}R_{n+1}(x) + \frac{4(n^2+19n/9+1)}{(3n+2)(3n+4)}R_n(x) \\
&\quad + \frac{4n(27n^2-16)}{9(3n-2)(3n+2)^2}R_{n-1}(x) + \frac{4n(n-1)}{3(3n-2)(3n+2)}R_{n-2}(x) \text{ if } n \text{ is even,} \\
&= \frac{4(n+1)}{9(3n+1)}R_{n+1}(x) + \frac{4(9n^2-n-1)}{9(3n-1)(3n+1)}R_n(x) + \frac{4n^2}{3(n+1)(3n+1)}R_{n-1}(x) \\
&\qquad + \frac{4n(n-1)^2}{3(3n-1)(3n+1)(n+1)}R_{n-2}(x) \text{ if } n \text{ is odd.}
\end{aligned} \tag{17}$$

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

```
v^{(0)} = [ 1 -1/2            0           0       0    0  0 ... ]
v^{(1)} = [ 0 7/72  -11/144   -1/40       0       0    0  0 ... ]
v^{(2)} = [ 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.

Classical multiple orthogonal polynomials through the Sonine-Hahn criterium (the derivatives of the polynomials being multiple orthogonal polynomials themselves) have been studied by Douak & Maroni [23]. See also Van Assche & Coussement [93] for another approach.

6. Weights with logarithmic singularities. Interior singularity.

6.1. **Known results.**

The influence of an algebraic singularity at $c \in (a,b)$ on the recurrence coefficients has been discussed in [29,63,65], it has been observed, and sometimes proved, that

$$\begin{aligned}
a_n - a_\infty &= f_n\cos(2n\theta_c+\varphi_c) + o(f_n), \\
b_n - b_\infty &= 2f_n\cos((2n+1)\theta_c+\varphi_c) + o(f_n),
\end{aligned} \tag{18}$$

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_c 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,

$$\begin{aligned}
&w(x) \approx w(c) + \text{constant } |x-c|^\alpha, \alpha > 0, 0 < w(c) < \infty \\
&\quad \Rightarrow f_n = \text{constant } n^{-\alpha-1},
\end{aligned} \tag{19}$$

see [63, p.156], first part of [65].

The proof in [63] makes heavy use of Toeplitz determinants based on Szegő's theory. The subsections 6.3-6.5 that will follow here try to suggest simpler approaches. No new proof will be presented, but the puzzling fact is that the form (18) holds for all kinds of interior singularities encountered up to now, whether as proved results, or as conjectures.

In the much more difficult situation where $w(c) = 0$ or ∞, the power of n in f_n does not depend on α, but we know

$$w(x) \sim \text{constant } |x-c|^{\alpha}, \alpha > -1 \Rightarrow f_n = -(b-a)|\alpha|/(8n), \tag{20}$$

[29, 65].

The brilliant proof of [29] uses new Riemann-Hilbert techniques.

Initially a way to reconstruct systems of differential equations from the properties of the solutions about their branchpoints (monodromy matrix), "the Riemann-Hilbert method reduces a particular problem to the reconstruction of an analytic function from jump conditions", in the words of A. Its [51, p. 1389]. The method has been applied with striking results to orthogonal polynomials asymptotics [51, p. 1391] [4, 22, 27, 53, 54], up to, as already noted, the proof of conjectures on interior singularities [29, 30].

At first, one looks [66, §3,4] at a transformation

$$\begin{bmatrix} P_n(x) & Q_n(x)/w(x) \\ P_{n-1}(x) & Q_{n-1}(x)/w(x) \end{bmatrix}_{\text{after}} = \begin{bmatrix} P_n(x) & Q_n(x)/w(x) \\ P_{n-1}(x) & Q_{n-1}(x)/w(x) \end{bmatrix}_{\text{before}} \begin{bmatrix} 1 & C_1 \\ 0 & C_2 \end{bmatrix}$$

with suitable C_1, C_2, around endpoints or singular points, with a very subtle scale dilation in some regions, this is the new feature found in present day developments of the Riemann-Hilbert method [4, 22, 27, 29, 30, 53, 54].

In the year 2000, Lubinsky wrote illuminating remarks on the virtues of various techniques, see here a (slightly shortened) part of the conclusion of his survey: " At present it seems that the Deift-Fokas-Its-Kitaev-Kriecherbauer- McLaughlin & al. method [= the new RH] will lead to very precise asymptotics for restricted classes of weights, while I believe that BernsteinSzegő-Rakhmanovs one will lead to asymptotics for more general weights, but with weaker error estimates. " [62, p. 251].

6.2. **Conjecture.** *If the weight function has one or several logarithmic singularities of the form $w(x) \sim$ constant $\times \log|x-c|$ near one or several values of $c \in (a, b)$, the main asymptotic behaviour of the related amplitude in* (18) *is*

$$f_n = \frac{(b-a)\sin\theta_c}{8n\log n}, \tag{21}$$

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

One has also $(b-a)\sin\theta_c = 2\sqrt{(c-a)(b-c)}$. As a matter of fact, the validity of this formula in the numerator of f_n is the weakest part of the conjecture, and may be wrong.

The conjecture 6.2 is motivated by interesting solid-state problems in §8, where weight functions with logarithmic singularities are encountered, and numerical results are seen in Tables 4 and 6.

6.3. About the Szegő asymptotic formula.

Warning: up to the end of the present section 6, I develop some ideas on the origin of the formulas (18), trying to show in several ways how they are related to the Szegő's theory.

No new proof follows, alas, but perhaps valuable work will be inspired by what follows.

The Szegő's theory is centered on 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 [88, chap. 12], also in the surveys by Lubinsky [61, 62] and Nevai [74], and in Van Assche's book [90, §1.3.1] the formula for the orthonormal polynomial is

$$p_n(x) \approx (2\pi)^{-1/2}[z^n \exp(\lambda(z^{-1})) + z^{-n} \exp(\lambda(z))], \tag{22a}$$

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 (22a) is exact for $n > d/2$ (Bernstein-Szegő class [62, § 2.1]). For a general weight in the Szegő class, the two sides of (22a) tend to be equal in some L_2 norm [62, eq. (12)] etc.

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

$$q_n(x) \approx (2\pi)^{1/2} \frac{4}{b-a} \frac{\exp(-\lambda(z^{-1}))}{z^n(z-z^{-1})}, \tag{22b}$$

see Barrett [7], also Van Assche [90, §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 (22a). 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 (22a)-(22b), then $p_n(x) \approx p_n^{(0)}(x) = \kappa_n^{(0)} x^n + \kappa_n'^{(0)} x^{n-1} + \cdots$, and

$$\kappa_n^{(0)} = \frac{\exp(\lambda_0/2)}{\sqrt{2\pi}\,(a_\infty)^n}, \quad \frac{\kappa_n'^{(0)}}{\kappa_n^{(0)}} = -nb_\infty + a_\infty\lambda_1. \tag{23}$$

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 $\|P_n\|^2 = \mu_0 a_1^2 \cdots a_n^2$:

$$\kappa_n = \frac{1}{\sqrt{\mu_0}\,a_1\cdots a_n}, \qquad \frac{\kappa_n'}{\kappa_n} = -b_0 - \cdots - b_{n-1}. \tag{24}$$

Each term of (24) behaves like the corresponding term of (23) when $n \to \infty$.

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

$$p_n(x)/\kappa_n = a_\infty^n z^n + a_\infty^{n-1}(nb_\infty - b_0 - \cdots - b_{n-1})z^{n-1} + \cdots \tag{25}$$

We have gathered useful asymptotic material, and try to see how it allows to explain the formulas (18).

First, a quick check of (22a): $\int_a^b p_n(x)p_m(x)w(x)dx \approx \int_a^b p_n^{(0)}(x)p_m^{(0)}(x)w(x)dx$
$= \dfrac{1}{2\pi}\int_a^b [z^n \exp(\lambda(z^{-1})) + z^{-n}\exp(\lambda(z))][z^m \exp(\lambda(z^{-1})) + z^{-m}\exp(\lambda(z))]$
$\dfrac{\exp(-\lambda(z)-\lambda(z^{-1}))dx}{a_\infty|z-z^{-1}|}$. 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 $\exp(\lambda(z)-\lambda(z^{-1}))$.

The same technique is now used in order to get these high index coefficients, and how they enter the following estimate of recurrence coefficients finer asymptotics:

$$a_n - a_\infty \approx \frac{a_\infty}{2}(\psi_{-2n+2} - \psi_{-2n}), \quad b_n - b_\infty \approx a_\infty(\psi_{-2n+1} - \psi_{-2n-1}), \tag{26}$$

where the ψs are the Fourier coefficients of

$$\psi(e^{i\theta}) = \exp(\lambda(e^{-i\theta}) - \lambda(e^{i\theta})) = \sum_{-\infty}^{\infty} \psi_k e^{ik\theta}. \tag{27}$$

The formula (26) has been established by a long and painful proof through Toeplitz determinants in [63, 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). It is wondered here if we can reach (26) more easily, and if these formulas still hold for stronger singularities, but to which strength?

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*[4], 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 (23) and (24):

$$\sqrt{\frac{\mu_0 e^{\lambda_0}}{2\pi}}\,\frac{a_1\cdots a_n}{a_\infty^n} - 1 \sim -\frac{\psi_{-2n}}{2}, \quad b_0 + \cdots + b_{n-1} - nb_\infty + a_\infty\lambda_1 \sim -a_\infty\psi_{-2n+1}. \tag{28}$$

Can we find a quick and dirty argument for (26) and (28)?

6.3.1. *From orthogonal polynomials coefficients.* 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 (22a). We take a better look at the integral $\int_a^b (p_n^{(0)}(t))^2 w(t)dt =$ $\dfrac{1}{4\pi i}\oint [z^{2n}\exp(\lambda(z^{-1})-\lambda(z)) + 2 + z^{-2n}\exp(\lambda(z)-\lambda(z^{-1}))]\dfrac{dz}{z} = 1 + \psi_{-2n}/2 +$ the half of the coefficient of $\exp 2ni\theta$ in the complex conjugate $\overline{\psi(e^{i\theta})}$ which is $\psi_{-2n}/2$ again. We now need $\kappa_n^{(0)}$, already estimated in (23), but we need again a refined estimation. The coefficient of x^n in $p_n^{(0)}$ 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

[4] D itself is an *outer* function [40, § 8], [62, p.211].

part of the argument is very weak), and we get refined $\kappa_n^{(0)}$ = the $\kappa_n^{(0)}$ of (23) 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 (28). 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 $p_{n-1}^{(0)} = \dfrac{1}{4\pi i}\displaystyle\oint [z^{2n-1}\exp(\lambda(z^{-1})-\lambda(z))+z+1/z+z^{-2n+1}\exp(\lambda(z)-\lambda(z^{-1}))]\frac{dz}{z} = \psi_{-2n+1}$ as seen before in similar situations, and the second part of (28) follows.

This way to get (28) is far from being a valuable proof! 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 of the numerical credibility of (26), actually of the first part of (28): 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 (28).

n	0	1	2	3	4	5	...	10
a_n		0.77414	0.43434	0.52081	0.49034	0.50548		0.49893
λ_{2n}	-0.63662	-0.21221	0.042441	-0.01819	0.01011	-0.00643		0.00160
ψ_{2n}	0.95317	0.21745	-0.022831	0.01252	-0.00738	0.00489		-0.00134
ψ_{-2n}	0.95317	-0.19755	0.058329	-0.02507	0.01353	-0.00838		0.00191
$2M_n-2$		0.23899	-0.055036	0.02590	-0.01325	0.00851		-0.00189

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

We see that the relevant information is indeed contained in the ψ_{-2n} coefficients of (27).

6.3.2. *From scattering theory.* An alternate source of knowledge is therefore most welcome: Van Assche gave in [91] a survey on how Case, Geronimo, and Nevai (and himself too, see [76]) investigated the relation between recurrence coefficients and weight function modification, by introducing a function $\phi(x) = \lim\limits_{n\to\infty}\dfrac{(z-z^{-1})P_n(x)}{a_\infty^n z^{n+1}}$ 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 [91] that

$$\phi(x) = 1 - \sum_0^\infty \left[\frac{b_n-b_\infty}{a_\infty z^{n+1}} + \frac{a_{n+1}^2-a_\infty^2}{a_\infty^2 z^{n+2}}\right]\frac{P_n(x)}{a_\infty^n} \tag{29}$$

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 (29) 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 (22a) and (23), $P_n(x)/(a_\infty z)^n = p_n(x)/(\kappa_n a_\infty^n z^n)$ 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 (26) .

6.3.3. *From recurrence relations as matrix products.* An interesting exercise is also to recover (22a-22b) from (26) by working a linearization of a product of 2×2 matrices containing the recurrence coefficients: $\begin{bmatrix} p_{N-1}(x) & q_{N-1}(x)\\ p_N(x) & q_N(x)\end{bmatrix}$
$=\displaystyle\prod_{n=0}^{N-1}\begin{bmatrix} 0 & 1\\ -a_{N-1-n}/a_{N-n} & (x-b_{N-1-n})/a_{N-n}\end{bmatrix}$ times $\begin{bmatrix} 0 & \sqrt{\mu_0}/a_0\\ 1/\sqrt{\mu_0} & S(x)/\sqrt{\mu_0}\end{bmatrix}$ ([70]), and we use $(A+E_{N-1})(A+E_{N-2})\cdots(A+E_0)\approx A^N+\displaystyle\sum_{n=0}^{N-1}A^{N-1-n}E_nA^n$, 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!

6.4. **Relation with Fourier coefficients asymptotics.**

So, (26)-(28) relates recurrence coefficients asymptotics to Fourier coefficients of large index, a well worked subject.

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 [59, p. 8, p.43, p.72], where $\hat f$ is the Fourier transform[5] 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 [26, §2.8], and Zygmund [100, 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 [100, chap.5, §2.6 and 2.24], so, the $1/n^{\alpha+1}$ is kept unchanged up to the ψ_ns and (19) is confirmed.

[5]The Fourier transform in Lighthill's book is written with kernel $\exp(-2\pi ixy)$.

Stretching the argument for weak singularity to a strong singularity such as $w(t) \sim$ constant $|t-c|^\alpha$ near c, the logarithm of w behaves like $\alpha \log|\cos\theta - \cos\theta_c| =$ constant $+\alpha$ 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 (20).

So, (26)-(28) *hold for weak singularities* $0 < w(c) < \infty$ *as they should, but fail for at least one important class of strong singularities* $w(c) = 0$ *or* ∞*.*

Remind that the correct result has been established through the new Riemann-Hilbert method [29, 30].

And what about a logarithmic singularity of the conjectures of §5.2-6.2, as encountered with $2-$dimensional crystals?

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

Now, in the case of conjecture 6.2, $\log w(t)$ has a $\log\log$ singularity! There is probably not much literature on Fourier coefficients of a $\log(\log|t-c|)$ singularity, but Zygmund [100, chap. 5, §2.31] and Wong & Lin [97] 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 § 8.

6.5. 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 [100, § 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 [30] can be the basis for a proof of the conjecture 6.2.

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.

7. About matrices in solid-state physics.

7.1. 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 and even superconductivity, magnetization... The description of the behaviour of such a system is achieved by a complex-valued function (called a wavefunction, which will simply be denoted as a *state* hereafter) of the time variable and d space variables, with $d = 1, 2$, or 3 according to our present knowledge of the world. The measure of some physical properties (*observables*), such as the magnetization, is the value of an appropriate linear functional or operator acting on the current state. At any given time, the states are to be found in a subset of $L^2(\mathbb{R}^d)$. This formidable set of functions[6] is often approximated by the set of linear combinations of a finite set of simple "atomic functions" with a small support around each site, quite similar to finite elements constructions.

A state is therefore a vector $\boldsymbol{u}$ of, say, N elements representing the relative weight of the sites in the decomposition of the wavefunction. Actually, the state depends on the time t and satisfies the Schrödinger equation

$$\frac{d\boldsymbol{u(t)}}{dt} = -\frac{i}{\hbar}\boldsymbol{H}\boldsymbol{u}(t), \tag{30}$$

where $\boldsymbol{H}$ is a real symmetric matrix of order N approximating the relevant one-particle Hamiltonian operator of the system. The (m,n) element of $\boldsymbol{H}$ describes the coupling of energy between sites m and n (self-coupling if $m = n$). This coupling decreases fast if m and n are far apart, and one often considers only nearby values (closest neighbour approximation, or tight-binding approximation see Economou's book [25, §5.2]) also the first pages of Giannozzi & al. [39] and Haydock [45, 46]).

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. If all the interactions between nearest neighbours are identical, we have

$$\boldsymbol{H} = \begin{bmatrix} \ddots & \ddots & \ddots & & & & \\ & \alpha & \beta & \alpha & & & \\ & & \alpha & \beta & \alpha & & \\ & & & \alpha & \beta & \alpha & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix} \tag{31}$$

In this case like in more realistic systems, 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).

When the Hamiltonian operator is independent of time, the Schrödinger equation (30) is solved by

$$\boldsymbol{u}(t) = \exp(-it\boldsymbol{H}/\hbar)\boldsymbol{u}(0) = \sum_{r=0}^{\infty} \frac{(-it\boldsymbol{H})^r \boldsymbol{u}(0)}{r!\hbar^r}, \tag{32}$$

Starting with an initial state vector $\boldsymbol{u}(0)$.

Equation of motion method [45, §34]: we examine the diffusion of an electron initially localized on some site, say the m^{th} one, at $x = x_m$, therefore described by a vector $\boldsymbol{u}(0)$ with a single nonzero element. By applying the evolution operator (32) to this initial state, we have to look at the m^{th} column of a combination of powers of the matrix $\boldsymbol{H}$.

On the one-dimensional example given by (31) when $\beta = 0$, the elements of the powers of $\boldsymbol{H}$ are Laurent coefficients of the same powers of $\alpha z^{-1} + \alpha z$ (symbol of a Toeplitz matrix [64, § 3 and 5]). So, from the binomial theorem, the diagonal element of $\boldsymbol{H}^{2r}$ is $\binom{2r}{r}\alpha^{2r} = \frac{(2r)!}{(r!)^2}\alpha^{2r}$ and (32) is $\sum_{r=0}^{\infty} \frac{(-i\alpha t)^{2r}}{(r!)^2\hbar^{2r}} = J_0(2\alpha t/\hbar)$ at the diagonal element $n = m$, $i^{n-m} J_{n-m}(2\alpha t/\hbar)$ [52, Chap. IX] at the n^{th} element of the lattice, or, with $x = x_m + (n-m)\ell$, and reinstating β through multiplication by $e^{-i\beta t/\hbar}$,

$$\boldsymbol{u}(t)_n = e^{-i\beta t/\hbar} i^{n-m}\, J_{|x_n - x_m|/\ell}(2\alpha t/\hbar). \tag{33}$$

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

See [84] for what seems similar calculations, perhaps in [85] too.

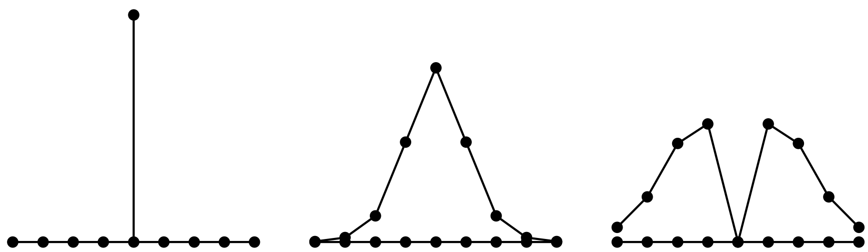

FIGURE 1. Diffusion of a single site occupation in a one-dimensional lattice.

Fig. 1 shows absolute values of components of a state vector $\boldsymbol{u}(t)_{m-4}, \ldots, \boldsymbol{u}(t)_{m+4}$ at various time values, starting with $\boldsymbol{u}(0)_n = \delta_{n,m}$. The last time value is such that $2\alpha t/\hbar = 2.404825\ldots$, the first zero of J_0 [1, p. 409] [52, IX, Table 32a]. Only the values on the lattice are relevant, the linear interpolation in Fig. 1 has no special meaning.

7.2. **Density of states.**

We now apply (32), using the eigenvalues and eigenstates $(E_p, \boldsymbol{v}^{(p)})$ of the simplified Hamiltonian operator $\boldsymbol{H}$. We now have

$$\boldsymbol{u}(t) = \sum_p \exp(-itE_p/\hbar)(\boldsymbol{v}^{(p)}, \boldsymbol{u}(0))\ \boldsymbol{v}^{(p)}, \tag{34}$$

where $(\boldsymbol{v}^{(p)}, \boldsymbol{u}(0))$ is the usual (complex) scalar product of the two vectors $\boldsymbol{v}^{(p)}$ and $\boldsymbol{u}(0)$).

We consider the projection $\boldsymbol{u(t)}_n$ on the n^{th} site starting from the m^{th} site, and rearrange the sum $\sum_p \exp(-itE_p/\hbar)\overline{\boldsymbol{v}_m^{(p)}}\boldsymbol{v}_n^{(p)}$, 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 $|\boldsymbol{v}_n^{(p)}|^2$ for the eigenvalues E_p in an interval of length dE around E. The result $n_{n,n}(E)dE$, where $n_{n,n}(E)$ is called the (local) *density of states*.

In the example (31), the eigenvalues are $E_p = \beta + 2\alpha\cos(p\pi/N)$ if the matrix has N rows & columns; normalized eigenvectors are $\boldsymbol{v}_n^{(p)} = \sqrt{2/N}\ \sin(np\pi/N)$ (average value of the sine squares is 1/2), see [42, chap. 7], [45, §12] .

In our example, starting from the m^{th} site, at $x = x_m = m\ell$, (34) becomes at the n^{th} site at time t

$$\begin{aligned} \boldsymbol{u}(t)_n &= 2\sum_p \exp(-it[\beta + 2\alpha\cos(p\pi/N)]/\hbar)\ \sin(mp\pi/N)\sin(np\pi/N)/N \\ &\sim (2/\pi)\int_0^\pi \exp(-it(\beta + 2\alpha\cos\theta))\sin(\theta x_m/\ell)\sin(\theta x_n/\ell)d\theta \end{aligned} \tag{35}$$

when we let $N \to \infty$ (continuous spectrum), with $x = n\ell, \theta = p\pi/N$.

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* [25,39,44–46,77]

$$G_{m,n}(x) = \int_a^b \frac{n_{m,n}(t)\,dt}{x - t} = ((x\boldsymbol{I} - \boldsymbol{H})^{-1})_{m,n},$$

which, if $m = n$, have the properties of the Stieltjes functions of the first section!

In the example above, (35) becomes at $x = n\ell$,

$$\begin{aligned} \boldsymbol{u}(t)_n &= \frac{1}{\pi}\int_0^{\pi} \exp(-it(\beta + 2\alpha\cos\theta)/\hbar)[\cos(\theta(x_n - x_m)/\ell) - \cos(\theta(x_n + x_m)/\ell)]d\theta \\ &= e^{-it\beta/\hbar}\left[i^{m-n} J_{n-m}(-2\alpha t/\hbar) - i^{m+n} J_{n+m}(-2\alpha t/\hbar)\right. \end{aligned}$$

[1, §9.1.21] [78, §10.9.2], where we recover (33), considering that $J_{n+m} \to 0$ when n and m are large: we only consider $x = x_n$ close to x_m.

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

Let $\boldsymbol{u}^{(0)}$ be a state represented by a vector of $\mathbb{R}^N$ (only the space variables are considered now), 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 $\boldsymbol{H}\boldsymbol{u}^{(n)} = a_n\boldsymbol{u}^{(n-1)} + b_n\boldsymbol{u}^{(n)} + a_{n+1}\boldsymbol{u}^{(n+1)}$:

$$\boldsymbol{H}[\boldsymbol{u}^{(0)} \mid \boldsymbol{u}^{(1)} \mid \boldsymbol{u}^{(2)} \mid \cdots] = [\boldsymbol{u}^{(0)} \mid \boldsymbol{u}^{(1)} \mid \boldsymbol{u}^{(2)} \mid \cdots] \begin{bmatrix} b_0 & a_1 & & & \\ a_1 & b_1 & a_2 & & \\ & a_2 & b_2 & a_3 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \tag{36}$$

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 $a_n = (\boldsymbol{u}^{(n-1)}, \boldsymbol{H}\boldsymbol{u}^{(n)}), b_n = (\boldsymbol{u}^{(n)}, \boldsymbol{H}\boldsymbol{u}^{(n)})$ [35, § 3.1.7.1] [41, chap. 9].

The recursion method has been, and still is, quite an inspiration in solid-state physics! [32, 39, 45–47]. 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.

7.4. **Perfect crystals.**

A perfect crystal is the repetition of a $d-$dimensional cell of atoms along d vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_d$ [73].

If there is a large but finite number of atomic positions (sites), the Hamiltonian operator is a large matrix acting on a vector $v(x_1, \ldots, x_d)$ as $\boldsymbol{H}v$ at the available site $(x_1, \ldots, x_d) = \sum_m h_m v(x + \delta_m)$, where each δ_m is a vector relating x to one of its neighbours in its cell and neigbouring cells. See the next section for two examples.

Let us try a vector $\exp(ik \cdot x) = \exp(i(k_1x_1 + \cdots + k_dx_d))$. The product by $\boldsymbol{H}$ 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 $\boldsymbol{H}$, for various real nonequivalent vectors k (Brillouin zone [39, §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 $\boldsymbol{H}$ (Grenander & Szegő [43, chap. 5,6, and notes of chap. 5])! More technically, $\boldsymbol{H}$ of a perfect crystal is a block-Toeplitz matrix with a matrix symbol.

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 $\mathrm{trace}((x\boldsymbol{I} - \boldsymbol{H})^{-1}) = \sum \dfrac{1}{x - E_p} = N \displaystyle\int_{E=h(k)=t} \dfrac{d\mathcal{N}(t)}{x-t} = N \int_{k\in B} \dfrac{|dk|}{x-h(k)}$ with the Brillouin zone B.

So, there is no need to estimate numerically the density of states of a perfect 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.

8. Two famous 2-dimensional lattices.

8.1. **The square lattice.**

The four vectors relating a site to its neighbours are $(\pm\ell, 0), (0, \pm\ell)$, see fig. 2, 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).

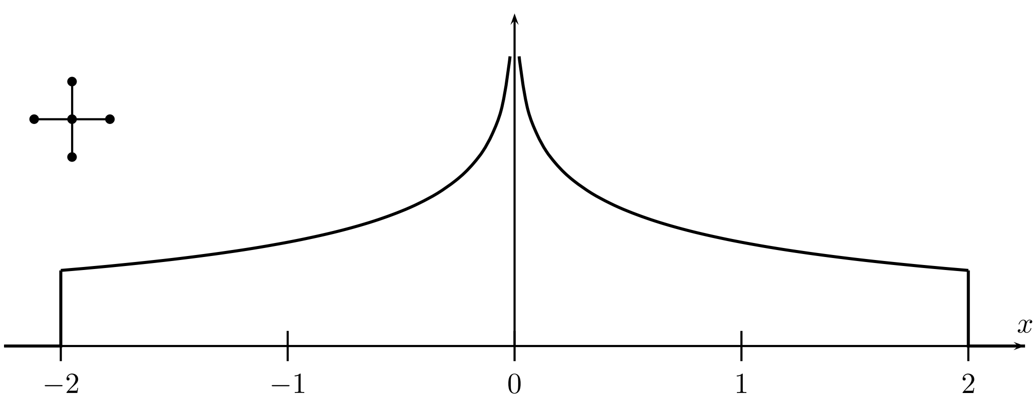

Figure 2. Square lattice: nearest neighbours and density of states.

Then (Economou [25, §5.3.2]),

$$S(x) = G_{0,0}(x) = (\pi)^{-2} \int_0^\pi \int_0^\pi \frac{dk_1\, dk_2}{x - \cos k_1 - \cos k_2} = \frac{2}{\pi x} \boldsymbol{K}\left(\frac{2}{x}\right), \tag{37}$$

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, so as to have $S(x) \sim 1/x$ for large x, unity as total weight).

Indeed, we integrate in k_2 for a given k_1, seeing that the integral from 0 to π is 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 (Borwein [10, §2.7], Jahnke & Emde [52, chap. V, C, §2.2], NIST [78, §19.8]), whence the result (37).

When x is real outside $[-2,2]$, $\boldsymbol{K}$ has an argument in $(-1,1)$ in (37) and is real there. When $x\in[-2,2]$, $\dfrac{2}{\pi x}\boldsymbol{K}\left(\dfrac{2}{x}\right) = \dfrac{1}{\pi}\displaystyle\int_0^{x/2}\dfrac{dr}{\sqrt{(1-r^2)(x^2/4-r^2)}} \pm \dfrac{i}{\pi}\int_{x/2}^1 \dfrac{dr}{\sqrt{(1-r^2)(r^2-x^2/4)}} = \dfrac{\operatorname{sign} x}{\pi}\boldsymbol{K}(x/2) \pm \dfrac{i}{\pi}\boldsymbol{K}(\sqrt{1-x^2/4})$ so[7], the weight function is [25, eq. 5.39])

$$w(x) = (1/\pi^2)\boldsymbol{K}(\sqrt{1-x^2/4}), \quad -2\leqslant x\leqslant 2. \tag{38}$$

Near $x=0$, using $\boldsymbol{K}(1-\varepsilon)\sim(1/2)\log(8/\varepsilon)$ (from [1, 17.3.26] with $m_1 = 1-(1-\varepsilon)^2$), the density of states has a $(\log(\sqrt{32}/|x|))/\pi^2$ behaviour near the origin.

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 $\boldsymbol{K}$ [78, §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

[7] use the change of variable $r^2 = 1-(1-x^2/4)s^2$ for the second integral.

negative powers of $z = x/2 + \sqrt{x^2/4-1}$, from (15). By a stroke of luck, $z = 1/\alpha$ used in the proof of (37), so we return to an intermediate result $S(x) = 2/(\pi z)\boldsymbol{K}(z^{-2})$ and apply (15) $\nu_0 + \sum_1^\infty \frac{2\nu_n}{z^n} = \frac{2(z-z^{-1})}{\pi z}\boldsymbol{K}(z^{-2})$, whence $\nu_0 = 1, \nu_2 = -1/2$, and

$$\nu_{4n} = -\nu_{4n+2} = \frac{1}{2^{2n+1}}\left(\frac{1\times 3\times\cdots(2n-1)}{n!}\right)^2, n = 1, 2, \ldots \tag{39}$$

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 (18) being thought to decrease like $1/(n\log n)$ from conjecture 6.2, 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 6.2 expects the limit 1/2. A second degree extrapolation makes this guess even more credible.

The graph of the weight function in Fig. 2 is established from $\mp\pi w(x)$ = imaginary part of the limit of $S(x \pm \varepsilon i)$ (Sokhotskyi-Plemelj [49, §14.1]) for x in the spectrum. $S(x)$ is computed as $\cfrac{1}{x - b_0 - \cfrac{a_1^2}{x - b_1 - \ddots}}$ which diverges on the spectrum. This problem is solved by replacing $\cfrac{a_N^2}{x - b_N - \cfrac{a_{N+1}^2}{\ddots}}$ by $\cfrac{a_\infty^2}{x - b_\infty - \cfrac{a_\infty^2}{\ddots}} = a_\infty/z = [x - b_\infty - \sqrt{(x-a)(x-b)}]/2$ which has a well-defined imaginary part on the two sides of the spectrum $[a, b]$. This is the termination method of Haydock & Nex [47, 77], and Lorentzen, Thron, and Waadeland [19, 60, 89] going back to Wynn [98, 99]. Máté, Nevai, and Totik [69, 75] 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 (22a) 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 $p > 1$ [19, 60, 92].

Of course, the formulas (37) and (38) are considered too.

8.2. **Hexagonal lattice: *graphene*.**

Graphene is a two-dimensional hexagonal arrangement of carbon atoms, of extreme importance in theoretical and applied physics [16, 24, 55, 57].

One half of the sites (the "A" sites) of the hexagonal arrangement of fig. 3 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 [50, §3], Katsnelson [55, §1.2], $h_{A\to B}(k_1, k_2) = 2e^{ik_1/2}\cos(k_2\sqrt{3}/2) + e^{-ik_1}, h_{B\to A}(k_1, k_2) = 2e^{-ik_1/2}\cos(k_2\sqrt{3}/2) + e^{ik_1}$.

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 $\begin{bmatrix} 0 & h_{A\to B}(k) \\ h_{B\to A}(k) & 0 \end{bmatrix}$,

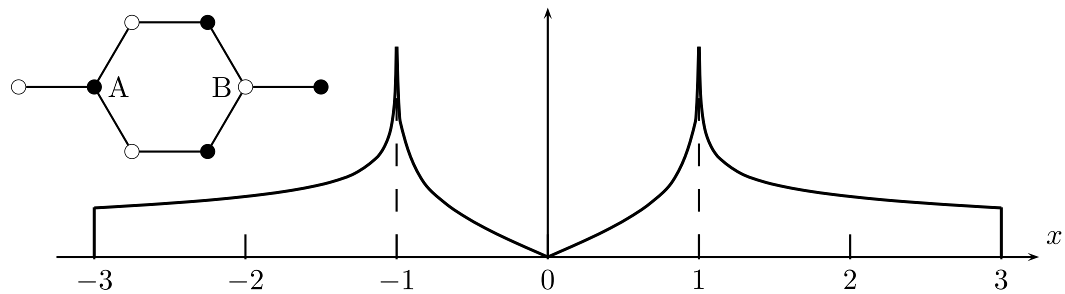

FIGURE 3. Graphene: nearest neighbors and density of states.

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

$$\begin{aligned} S(x) = G_{0,0}(x) &= \frac{1}{2\pi^2}\int_0^\pi\int_0^\pi \left[\frac{1}{x-E(\xi)} + \frac{1}{x+E(\xi)}\right] d\xi_1 d\xi_2 \\ &= \frac{x}{\pi^2}\int_0^\pi\int_0^\pi \frac{d\xi_1 d\xi_2}{x^2 - 4\cos^2\xi_2 - 4\cos\xi_1\cos\xi_2 - 1} \\ &= \frac{\sqrt{ux}}{\pi}\boldsymbol{K}(u), \text{ where } u = \frac{x^4 - 6x^2 - 3 - \sqrt{(x^2-1)^3(x^2-9)}}{8x}. \end{aligned} \tag{40}$$

The last formula [50] 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. 3 follow from the last line of (40) 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 $x = 1$, $u = -1 + i(x-1)^{3/2} + \cdots$, $\boldsymbol{K}(u) \sim \log(4/\sqrt{1-u^2}) \sim (-3/4)\log|x-1| +$ constant, [1, 17.3.26] [52, chap. V, §C.1 and 3], $S(x) \sim -(3i)/(4\pi)\log|x-1| +$ constant 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, 10, 78].

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 $[-3,3]$.

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 $\nu_6 = 47/243, \nu_8=-167/729, \nu_{10}=1013/6561$.

From (15), $\nu_0/2$ and $\nu_n, n>0,=$ the coefficients of z^{-n} of
$\dfrac{3(z-z^{-1})}{4} S\left(x = \dfrac{3(z+z^{-1})}{2}\right) = \dfrac{3(z-z^{-1})}{4}\left[\dfrac{2}{3(z+z^{-1})} + 3\left(\dfrac{2}{3(z+z^{-1})}\right)^3+\cdots\right] = \dfrac{1}{2} - \dfrac{1}{3z} + \ldots$

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.* [79,80] 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 [72, chap. 15], Bender & Orszag [9, § 3.2, 3.3], Andrews & al. [2, App. F]). 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 $c_{n+\delta}, \ldots, c_{n-d}$. Chebyshev expansions themselves are considered by Fox & Parker [31, Chap. 5].

We apply this programme to the coefficients of the expansion

$$3(z - z^{-1})S(x)/4 = 3(z - z^{-1})\sqrt{ux}\boldsymbol{K}(u)/(4\pi) = \frac{\nu_0}{2} + \sum_{n=1}^{\infty} \frac{\nu_{2n}}{z^{2n}} \tag{41}$$

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, $u(1-u^2)d^2\boldsymbol{K}/du^2 + (1-3u^2)d\boldsymbol{K}/du - u\boldsymbol{K} = 0$ [78, § 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

$$u^{\pm 1} = \frac{27z^4 + 36z^2 + 2 + 36z^{-2} + 27z^{-4} \mp (z - z^{-1})(9z^2 + 14 + 9z^{-2})^{3/2}}{64(z + z^{-1})} \tag{42}$$

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

$$\frac{du}{u\,dz} = \frac{(z^2-1)(9z^2 + 14 + 9/z^2)^2}{32(z^2+1)^2(u - u^{-1})} = -\frac{(9z^2 + 14 + 9/z^2)^{1/2}}{z^2+1}, \tag{43}$$

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 (15) and (40), 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 constant $(z - z^{-1})^{-1}(z + z^{-1})^{-1/2}S$

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

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

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}

$$9(n+3)^2\nu_{2n+6}+2(7n^2+35n+45)\nu_{2n+4}-9(n^2-2n-7)\nu_{2n+2}-4(7n^2-11)\nu_{2n}$$
$$-9(n^2+2n-7)\nu_{2n-2}+2(7n^2-35n+45)\nu_{2n-4}+9(n-3)^2\nu_{2n-6}=0, n=0,1,\ldots \quad (44)$$

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 $-1/3, -5/27, 47/243, -167/729, 1013/6561, -15653/177147, \ldots$ as already seen before, but the recurrence relation (44) 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 $S(x)\sim -(3i)/(4\pi)\log|x-1|+$ constant 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 (15): $(6/8)(z-1/z)S(x)\sim \pm(3\sqrt{2}/4\pi)\log(z\pm z_0^{\pm 1})$ 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. [95, §V.B.2, Table II]. See also Prevost [81] on weight reconstruction with Chebyshev moments.

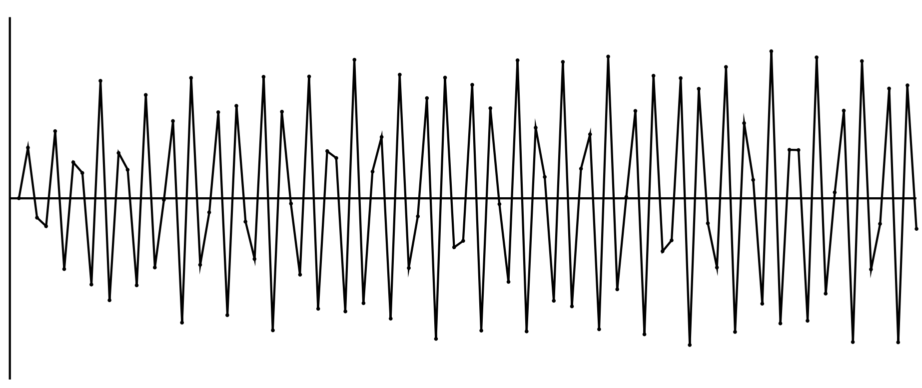

FIGURE 4. Graphene: 100 first $\rho_n=n\log n[a_n-3/2+(3/4)(-1)^n/n-(3/16)/n^2]$.

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 a constant 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

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., $\varphi/\pi, \rho_{n-1}/\rho_n$

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 $\cos(2\theta_c) = -7/9 = -0.7777\ldots$, checked in the last column of table 6 (the first approximated crest is at $n = 10$, see also Fig. 4), 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 6.2 amounts to expecting $\sqrt{2} = 1.414\ldots$ which is neither close nor far from the numerical estimate $1.405\ldots$

The first 69999 recurrence coefficients $a_1, \ldots, a_{69999}$ 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,
```

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