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The Constants in the Central Limit Theorem for the One-Dimensional Edwards Model

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The Edwards model in one dimension is a transformed path measure for one-dimensional Brownian motion discouraging self-intersections. We study the constants appearing in the central limit theorem (CLT) for the endpoint of the path (which represent the mean and the variance) and the exponential rate of the normalizing constant. The same constants appear in the weak-interaction limit of the one-dimensional Domb–Joyce model. The Domb–Joyce model is the discrete analogue of the Edwards model based on simple random walk, where each self-intersection of the random walk path recieves a penalty $e^{-2\beta}$. We prove that the variance is strictly smaller than 1, which shows that the weak interaction limits of the variances in both CLTs are singular. The proofs are based on bounds for the eigenvalues of a certain one-parameter family of Sturm–Liouville differential operators, obtained by using monotonicity of the zeros of the eigenfunctions in combination with computer plots.

KEY WORDS: Edwards model; Domb–Joyce model; central limit theorem; spectral analysis; Sturm–Liouville theory.

1. MOTIVATION AND MAIN RESULTS

1.1. The Edwards Model

Let $(B_t)_{t\geqslant 0}$ be standard one-dimensional Brownian motion starting at 0. Let $\hat{P}$ denote its distribution on path space and $\hat{E}$ the corresponding expectation. The *Edwards model* is a transformed path measure discouraging self-intersections, defined by the intuitive formula

$$\frac{d\hat{P}_T^\beta}{d\hat{P}}=\frac{1}{\hat{Z}_T^\beta}\exp\left[-\beta\int_0^T ds\int_0^T dt\,\delta(B_s-B_t)\right]\qquad (T\geqslant 0)\qquad (1.1)$$

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Here δ denotes Dirac's function, $\beta \in (0, \infty)$ is the *strength of self-repellence* and $\hat{Z}_T^\beta$ is the normalizing constant. A rigorous definition of $\hat{P}_T^\beta$ can be given in terms of Brownian local times, namely

$$\int_0^T ds \int_0^T dt\, \delta(B_s - B) = \int_{\mathbb{R}} dx\, L^2(T, x) \tag{1.2}$$

where $L(T, x)$ is the local time at x until time T. In van der Hofstad, den Hollander and König[5] a central limit theorem (CLT) is proved for the Edwards model. To formulate this we have to introduce some notation. For $a \in \mathbb{R}$, define $\mathscr{K}^a$: $L^2(\mathbb{R}_0^+) \cap C^2(\mathbb{R}_0^+) \to C(\mathbb{R}_0^+)$ by

$$(\mathscr{K}^a x)(u) = 2ux''(u) + 2x'(u) + (au - u^2)\, x(u) \qquad \text{for} \quad u \in \mathbb{R}_0^+ = [0, \infty) \tag{1.3}$$

The Sturm–Liouville operator $\mathscr{K}^a$ will play a key role in the present paper.[2] It is symmetric and has a largest eigenvalue $\rho(a)$ with unique positive and L^2-normalized eigen-function x_a. The map $a \mapsto \rho(a)$ is real-analytic, strictly convex and strictly increasing, with $\rho(0) < 0$, $\lim_{a \to -\infty} \rho(a) = -\infty$ and $\lim_{a \to \infty} \rho(a) = \infty$. Define $a^*, b^*, c^* \in (0, \infty)$ by

$$\rho(a^*) = 0, \qquad b^* = \frac{1}{\rho'(a^*)}, \qquad c^{*2} = \frac{\rho''(a^*)}{\rho'(a^*)^3} \tag{1.4}$$

Theorem 1 (van der Hofstad, den Hollander, and König[5]). For every $\beta \in (0, \infty)$

$$\lim_{T \to \infty} \hat{P}_T^\beta \left(\frac{|B_T| - b^* \beta^{1/3} T}{c^* \sqrt{T}} \leqslant C \right) = \int_{-\infty}^C \frac{e^{-x^2/2}}{\sqrt{2\pi}}\, dx \qquad \text{for all} \quad C \in \mathbb{R} \tag{1.5}$$

and

$$a^* \beta^{2/3} = -\lim_{T \to \infty} \frac{1}{T} \log \hat{Z}_T^\beta \tag{1.6}$$

The simple dependence on β of the mean, the variance and the exponential rate of the normalizing constant in Theorem 1 follows from Brownian scaling (see van der Hofstad, den Hollander, and König[5] Section 0.3).

[2] The operator $\mathscr{K}^a$ is a scaled version of the operator $\mathscr{L}^a$ originally analyzed in van der Hofstad and den Hollander[4] Section 5, namely $(\mathscr{K}^a x)(u) = (\mathscr{L}^a \bar{x})(u/2)$ where $\bar{x}(u) = x(2u)$.

1.2. The Domb–Joyce Model

Let $(S_i)_{i \in \mathbb{N}_0}$ be simple random walk on $\mathbb{Z}$, starting at the origin. Let E be expectation with respect to the simple random walk measure. Let P_n^β be the measure on n-step paths given by

$$\frac{dP_n^\beta}{dP} = \frac{1}{Z_n^\beta} \exp\left[-\beta \sum_{\substack{i,\, j=0 \\ i \neq j}}^{n} 1_{\{S_i = S_j\}} \right] \tag{1.7}$$

where Z_n^β is the normalizing constant. The Domb–Joyce model is a transformed path measure on the space of n-step paths as in (1.1), where the Wiener measure is replaced by the simple random walk measure and the exponent in (1.1) by the exponent in (1.7). It is therefore the discrete analogue of the Edwards measure. The Domb–Joyce measure gives a penalty $e^{-2\beta}$ for every self-intersection of the path.

We have the following CLT, similar to Theorem 1:

Theorem 2. For every $\beta \in (0, \infty)$, there exist $\theta^*(\beta), \sigma^*(\beta) \in (0, 1]$, such that

$$P_n^\beta\left(\frac{|S_n| - \theta^*(\beta)\, n}{\sigma^*(\beta) \sqrt{n}} \leqslant C \right) = \int_{-\infty}^{C} \frac{e^{-x^2/2}}{\sqrt{2\pi}}\, dx \qquad \text{for all} \quad C \in \mathbb{R} \tag{1.8}$$

Furthermore, there exists $r^*(\beta) \in (0, \infty)$ such that

$$r^*(\beta) = -\lim_{n \to \infty} \frac{1}{n} \log Z_n^\beta \tag{1.9}$$

Moreover,

$$\lim_{\beta \downarrow 0} \beta^{-2/3} r^*(\beta) = a^* \tag{1.10}$$

$$\lim_{\beta \downarrow 0} \beta^{-1/3} \theta^*(\beta) = b^* \tag{1.11}$$

$$\lim_{\beta \downarrow 0} \sigma^*(\beta) = c^* \tag{1.12}$$

The results in Theorem 2 are taken from different papers. The law of large numbers is proved in Greven and den Hollander,[2] the central limit theorem in König.[7] The scaling of $r^*(\beta)$ and $\theta^*(\beta)$ is proved in van der Hofstad and den Hollander,[4] while the scaling of $\sigma^*(\beta)$ is in van der Hofstad, den Hollander, and König.[6]

The important message of Theorems 1 and 2 is that as β becomes small, the constants in the CLTs for the Edwards model and the Domb–Joyce model have the same scaling.

Since the standard deviation c^* in Theorem 1 is *independent* of β and c^* is the weak interaction limit of the standard deviation in Theorem 2, it is interesting to know whether c^* differs from 1, the standard deviation of free Brownian motion and simple random walk. In Theorem 3(a–c) below we will give bounds on the constants a^*, b^*, and c^*.

1.3. Main Theorem: Theorem 3

The following is our main theorem:

Theorem 3.

(a) $a^* \in [2.188, 2.189]$

(b) $b^* \in [1.104, 1.124]$

(c) $c^* \in [0.60, 0.66]$.

The proof of Theorem 3 is given in Sections 2–5 and is based on estimates of the eigenvalues of the differential operator $\mathscr{K}^a$ (recall (1.3)). Section 2 describes the Sturm–Liouville theory with which we can estimate the constants and which follows from Sturm–Liouville comparison theorems. In Sections 3–5 we derive the estimates for a^*, b^* and c^*, respectively. These estimates are computer-assisted and we give exact error estimates.

The bounds in Theorem 3(a–b) can be made arbitrarily sharp by making the estimates of the eigenvalues sharper. For the bound in Theorem 3(c) this is *not* the case, which is due to the fact that c^* in (1.4) is a more complicated object.

1.4. Discussion

Our main result is that the constant c^*, giving the standard deviation of the endpoint of the path in both the Edwards model and the weakly interacting Domb–Joyce model, is strictly smaller than 1.

This means that the variances in the CLTs for the Domb–Joyce model and the Edwards model are discontinuous $\beta = 0$ and that, as the path is pushed out to infinity on a linear scale, the fluctuations around the asymptotic mean are squeezed compared to the fluctuations of simple random walk, respectively, free Brownian motion. Indeed, for free simple random walk and free Brownian motion we have $E(S_n^2/n) = \hat{E}(B_T^2/T) = 1$

for all $n \in \mathbb{N}$ and $T > 0$. Intuitively, this is because the endpoint of the path lives on a larger scale as free Brownian motion and simple random walk, respectively. Therefore, we can think of the law of the endpoint of being less random, which implies that the variance is smaller.

2. PREPARATIONS: LEMMAS 1–4

In this section we shall analyze the zeros of the eigenfunctions of the Sturm-Liouville differential operator $\mathscr{K}^a$ (recall (1.3)).

Throughout the sequel, we will frequently refer to van der Hofstad and den Hollander[4] and van der Hofstad, den Hollander, and König.[6] We will therefore adopt the abbreviations HH and HHK for these references.

2.1. Sturm–Liouville Theory: Lemmas 1–3

Let $u \mapsto x_{a,\rho}(u)$ be the solution of

$$(\mathscr{K}^a x)(u) = 2ux''(u) + 2x'(u) + 2(au - u^2)\, x(u) = \rho x(u) \tag{2.1}$$

with $x_{a,\rho}(0) = 1$ and note that $x'_{a,\rho}(0) = \rho$ (see also HH Section 2.6). This solution is unique, since the origin is a regular singular point of (2.1) (see also HH Lemma 19 (i)), but by HH Lemma 20 it need not be in $L^2(\mathbb{R}_0^+)$! In fact, the only values of ρ for which $x_{a,\rho}$ is in $L^2(\mathbb{R}_0^+)$ are the eigenvalues $\rho^{(k)}(a)$ $(k = 0, 1,...)$, arranged in decreasing order with $\rho^{(0)}(a) = \rho(a)$ (see HHK Section 3.1). Define the corresponding normalized eigenfunctions to be $x_a^{(k)} = x_{a,\rho^{(k)}(a)}/\|x_{a,\rho^{(k)}(a)}\|_2$ (and note that $x_a^{(0)} = x_a$).

In the sequel we shall use the extreme sensitivity of the tails of $x_{a,\rho}$ with respect to a and ρ to get sharp numerical estimates for the eigenvalues $\rho^{(k)}(a)$.

Suppose that $u(a, \rho) < \infty$ is a zero of $x_{a,\rho}$. The starting point of our investigation is the following lemma:

Lemma 1. For all $a, \rho \in \mathbb{R}$ and $u(a, \rho) < \infty$,

$$\begin{aligned} &\frac{\partial}{\partial \rho} u(a, \rho) \geqslant 0 \\ &\frac{\partial}{\partial a} u(a, \rho) \leqslant 0 \end{aligned} \tag{2.2}$$

Proof. The lemma follows from Sturm–Liouville comparison theorems. See e.g., Coddington and Levinson,[1] p. 212, proof of

Theorem 2.1, where there is a proof for the regular case. The proof for the regular singular case is similar if we apply the results to $y_{a,\rho}(u) = x_{a,\rho}(u)/x_{a,\rho}(\varepsilon)$, where $\varepsilon > 0$ is so small that $x_{a,\rho}(u)$ has no zeros on $[0, \varepsilon]$. This proves that the zeros of $y_{a,\rho}$ are monotone on $[\varepsilon, \infty)$, which implies the lemma. ∎

Lemma 1 states that if there is a zero for $x_{a,\rho}$, then this zero will move to the left as ρ decreases or a increases and vice versa. Furthermore, $x_{a,\rho}(0) = 1$ prevents zeros from moving to the negative axis. Hence, $x_{a,\rho}$ can only get more zeros as ρ decreases or a increases.

From Lemma 1 follows a stronger statement:

Lemma 2. Let $n = n(a, \rho)$ be defined by

$$n(a, \rho) = \#\{\text{zeros of } x_{a,\rho}\} \tag{2.3}$$

Then, for every $a \in \mathbb{R}$, $\rho \mapsto n(a, \rho)$ is a step function that makes a jump precisely at the eigenvalues $\rho^{(k)}(a)$, i.e., $n(a, \rho) = k$ for $\rho \in [\rho^{(k)}(a), \rho^{(k-1)}(a))$ $(k \geqslant 0)$.

Proof. See Coddington and Levinson[1] Theorem 2.1 on p. 212, together with Lemma 1. ∎

Let

$$c(a, \rho) = \tfrac{1}{2}a + \tfrac{1}{2}\sqrt{a^2 - 4\rho} \tag{2.4}$$

be the last zero of $u^2 - au + \rho$.

Lemma 3. If $v \geqslant c(a, \rho)$ and if $x_{a,\rho}(v)$ and $x'_{a,\rho}(v)$ have the same sign, then $x_{a,\rho}(u)$ and $x'_{a,\rho}(u)$ have the same sign for all $u \geqslant v$.

Proof. Easy. See (2.1). ∎

Lemma 3 will be useful in order to determine the number of zeros of $x_{a,\rho}$ from a computer plot of $x_{a,\rho}(u)$ for u in a bounded interval.

2.2. Power Series Approximation: Lemma 4

We end this preparatory section by results that will allow us to determine the number of zeros of $x_{a,\rho}$ in a bounded interval.

Use HH (5.23) to write $x_{a,\rho}(u)$ as a power series

$$x_{a,\rho}(u) = \sum_{n=0}^{\infty} g_n u^n \tag{2.5}$$

where the g_n's satisfy the recurrence relation

$$g_n = \frac{1}{2n^2} (\rho g_{n-1} - a g_{n-2} + g_{n-3}) \qquad (n \geqslant 1) \tag{2.6}$$

with $g_0 = 1$, $g_{-1} = g_{-2} = 0$. By induction on n, it is easy to derive the following bounds:

$$|g_n| \leqslant \frac{K(a, \rho)^n}{(n!)^{2/3}} \qquad (n \geqslant 1) \tag{2.7}$$

where $K(a, \rho)$ satisfies

$$\frac{|\rho|}{2^{5/3} K(a, \rho)} + \frac{|a|}{2^{4/3} K(a, \rho)^2} + \frac{1}{2K(a, \rho)^3} \leqslant 1 \tag{2.8}$$

In the sequel we shall take

$$K(a, \rho) = \max \left\{ 2^{-2/3} |\rho|, \sqrt{\frac{3|a|}{2^{4/3}}}, \sqrt[3]{3} \right\} \tag{2.9}$$

(This corresponds to bounding the first term in (2.8) by $\frac{1}{2}$, the second by $\frac{1}{3}$ and the third by $\frac{1}{6}$. This choice turns out to be good enough for the choices of a and ρ that we will use in the sequel.)

In order to estimate how well the power series with a finite number of terms approximates $x_{a,\rho}(u)$ on a bounded u-interval, we have to know what the contribution is of the remote summands in (2.5).

Lemma 4. For every $k \in \mathbb{N}$, ρ, $a \in \mathbb{R}$ and $K \in \mathbb{R}^+$,

$$\left| \sum_{n=k}^{\infty} g_n u^n \right| \leqslant \frac{[NC_k]^k}{(1 - NC_k) \sqrt[3]{2\pi k}} \qquad \text{uniformly for} \quad u \in [0, N] \tag{2.10}$$

where C_k is given by

$$C_k = C_k(a, \rho) = \frac{K(a, \rho)\, e^{2/3}}{k^{2/3}} \tag{2.11}$$

Proof. Use Stirling's inequality

$$n! \geqslant \sqrt{2\pi n} \left(\frac{n}{e} \right)^n \tag{2.12}$$

and (2.7), to get

$$\text{l.h.s. } (2.10) \leqslant \sum_{n=k}^{\infty} \frac{[NC_n]^n}{\sqrt[3]{2\pi n}} = \sum_{n=0}^{\infty} \frac{[NC_{n+k}]^{n+k}}{\sqrt[3]{2\pi(n+k)}} \leqslant \frac{[NC_k]^k}{\sqrt[3]{2\pi k}} \sum_{n=0}^{\infty} [NC_k]^n \quad \blacksquare \tag{2.13}$$

We have now completed our preparation and can start with the proof of Theorem 3.

3. PROOF OF THEOREM 3(a)

Fix $\rho = 0$ and $N = 8$, $k = 350$. Use Lemma 2 to see that if $x_{a,0}$ has a zero then $a > a^*$, while if $x_{a,0}$ has no zero then $a \leqslant a^*$.

Next, (2.9) gives that

$$K(a, 0) \leqslant 1.7 \qquad \text{uniformly for} \quad a \leqslant 2.2 \tag{3.1}$$

Hence, in (2.11),

$$C_k \leqslant 0.07 \tag{3.2}$$

Thus, by (2.10), the difference of $x_{a,\rho}$ and the power series approximation of $x_{a,\rho}(u)$ with 350 terms is smaller than or equal to 2×10^{-89} (for these values of N, a, ρ and k).

The proof now follows from Fig. 1, Lemma 3 and the fact that $c(a, 0) = a < N = 8$ for $a \leqslant 2.2$ (recall (2.4)).

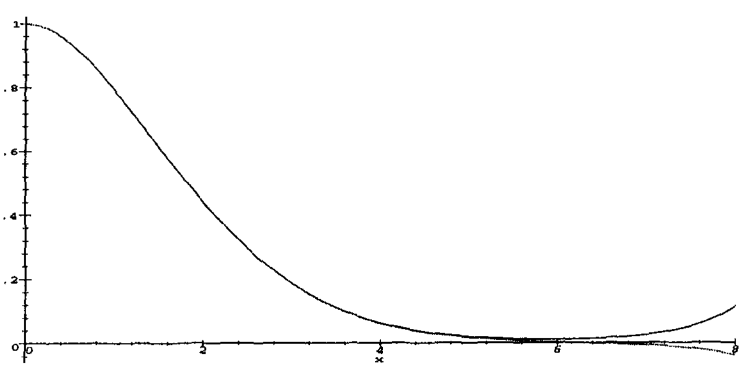

Fig. 1. The power series approximation of $x_{a,0}$ with $a = 2.188$, respectively $a = 2.189$ and $N = 8$, $k = 350$.

4. PROOF OF THEOREM 3(b)

4.1. The Lower Bound for b^*

First we derive an equality, (4.2) below, that we need later on to prove the lower bound for b^*.

Compute

$$0 = [ux'_{a^*}(u)]^2 |_0^\infty = 2 \int_0^\infty (ux'_{a^*}(u))' \, ux'_{a^*}(u) \, du$$

$$= -\int_0^\infty (a^*u - u^2) \, ux'_{a^*}(u) \, x_{a^*}(u) \, du \tag{4.1}$$

where we used (1.3) and $\rho(a^*) = 0$. Now, integrate by parts to get

$$0 = a^* \int_0^\infty ux^2_{a^*}(u) \, du - \frac{3}{2} \int_0^\infty u^2 x^2_{a^*}(u) \, du = \frac{a^*}{b^*} - \frac{3}{2} \int_0^\infty u^2 x^2_{a^*}(u) \, du \tag{4.2}$$

since

$$\rho'(a) = \int_0^\infty ux^2_a(u) \, du \tag{4.3}$$

(Note that the boundary terms at infinity disappear by the super-exponential decay of x_{a^*} in HH Lemma 20.)

To get the lower bound for b^*, use $(1/b^*) = \rho'(a^*)$ and recall (4.3) and write out using partial integration:

$$\begin{aligned} a^* - \frac{2}{b^*} &= \int_0^\infty du (a^*u - u^2)' \, x^2_{a^*}(u) \\ &= -2 \int_0^\infty du (a^*u - u^2) \, x_{a^*}(u) \, x'_{a^*}(u) \\ &= 4 \int_0^\infty du [x'_{a^*}(u)^2 + ux''_{a^*}(x) \, x'_{a^*}(u)] \\ &= 2 \, \|x'_{a^*}\|_2^2 \end{aligned} \tag{4.4}$$

Here the third equality uses (1.3), while the fourth equality again follows from partial integration.

Therefore, a rough lower bound for b^* is

$$a^* - \frac{2}{b^*} \geqslant 0 \qquad \text{or} \qquad b^* \geqslant \frac{2}{a^*} \tag{4.5}$$

which together with Theorem 3(a) gives

$$b^* \geqslant 0.91 \tag{4.6}$$

However, (4.6) can be improved using (4.2), partial integration and the Cauchy–Schwarz inequality:

$$\begin{aligned} 1 &= -2 \int_0^\infty du\, u x_{a^*}(u)\, x'_{a^*}(u) \\ &\leqslant 2\, \|x'\|_2 \sqrt{\int_0^\infty du\, u^2 x^2_{a^*}(u)} \\ &= \sqrt{2}\, \|x'\|_2 \sqrt{\frac{4}{3} \frac{a^*}{b^*}} \\ &= \frac{1}{b^*} \sqrt{a^* b^* - 2} \sqrt{\frac{4}{3} a^*} \end{aligned} \tag{4.7}$$

Rewrite this to get

$$a^* b^* - 2 \geqslant b^{*2} \frac{3}{4} \frac{1}{a^*} \tag{4.8}$$

or

$$b^* \geqslant \frac{2}{a^*} + b^{*2} \frac{3}{4} \frac{1}{a^{*2}} \tag{4.9}$$

Now, insert (4.6) into the r.h.s. of (4.9) and use Theorem 3(a) to get

$$b^* \geqslant 1.043 \tag{4.10}$$

Iterating (4.9) seven times, each time with the improved lower bound in the r.h.s., we arrive at the lower bound in Theorem 3(b).

4.2. The Upper Bound for b^*

To prove the upper bound for b^*, use the fact that $a \mapsto \rho'(a)$ is increasing, the relation $b^* = [\rho'(a^*)]^{-1}$ (see HH Theorems 5 and 6 and Theorem 3(a)), the mean value theorem and Theorem 3(a) to get that

$$b^* \leqslant \frac{1}{100[\rho(2.188) - \rho(2.178)]} \tag{4.11}$$

Furthermore, $c(a, \rho) \leqslant 3 < N = 9$ for these values of a, ρ (recall (2.4)), so that Lemma 3 applies. Recall (2.9) to get

$$K(a, \rho) \leqslant 1.7 \qquad \text{uniformly for} \quad \rho \in [-0.0096, 0], \quad a \in [2.178, 2.188] \tag{4.12}$$

Hence (2.11) gives

$$C_k(a, \rho) \leqslant 0.07 \qquad \text{uniformly for} \quad \rho \in [-0.0096, 0], \quad a \in [2.178, 2.188] \tag{4.13}$$

Thus, by (2.10), the difference between $x_{a,\rho}(u)$ and the power series approximation of $x_{a,\rho}(u)$ with 350 terms is smaller than or equal to 2×10^{-71} (for these values of N, a, ρ and k).

Now use Lemma 2 and Fig. 2 to get that

$$\begin{aligned} \rho(2.178) &\leqslant -0.0096 \\ \rho(2.188) &\geqslant -0.0007 \end{aligned} \tag{4.14}$$

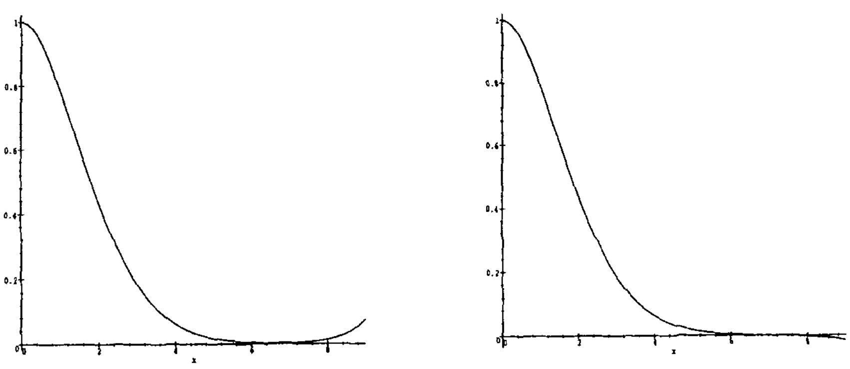

Fig. 2. The power series approximation of $x_{a,\rho}$ with $(a, \rho) = (2.188, -0.0096)$, respectively, $(a, \rho) = (2.178, -0.0007)$ and $N = 9, k = 350$.

since $x_{a,\rho}$ has one zero for $(a, \rho) = (2.187, -0, 0096)$ (note that $x_{a,\rho}(N) < 0$ for $(a, \rho) = (2.187, -0, 0096)$), while $x_{a,\rho}$ has no zero for $(a, \rho) = (2.177, -0, 0007)$ (note that $x_{a,\rho}(N) > 0$ for $(a, \rho) = (2.187, -0, 0007)$).

5. PROOF OF THEOREM 3(c)

In Sections 5.1 and 5.2 we prove the upper bound for c^*, in Section 5.3 the lower bound for c^*.

5.1. The Upper Bound for c^*: Lemmas 5 and 6

By differentiating (4.3) w.r.t. a, we get

$$\rho''(a) = 2 \int_0^\infty du\, u x_a(u)\, y_a(u) \tag{5.1}$$

where $y_a \in L^2(\mathbb{R}_0^+)$ is the function

$$y_a(u) = \frac{d}{da} x_a(u) \tag{5.2}$$

Differentiating the relation $\|x_a\|_2^2 = 1$ with respect to a, we get

$$\langle x_a, y_a \rangle_2 = 0 \tag{5.3}$$

Hence, we can rewrite (5.1) as

$$\rho''(a) = 2 \int_0^\infty du(u - \rho'(a))\, x_a(u)\, y_a(u) \tag{5.4}$$

Note that by (4.3) also $u \mapsto (u - \rho'(a))\, x_a(u)$ is orthogonal to x_a. Furthermore, differentiating the eigenvalue relation $\mathscr{K}^a x_a = \rho(a)\, x_a$ with respect to a, we get that y_a satisfies the inhomogeneous differential equation

$$-(\mathscr{K}^a y)(u) + \rho(a)\, y(u) = f_a(u) \tag{5.5}$$

where

$$f_a(u) = (u - \rho'(a))\, x_a(u) \tag{5.6}$$

HH Lemma 20 gives that all the $\rho^{(k)}(a)$'s have multiplicity 1. The Rayleigh representation for $\rho^{(1)}(a)$ reads

$$\rho^{(1)}(a) = \sup_{y:\, \|y\|_2 = 1,\, \langle x_a, y\rangle_2 = 0} \langle y, \mathscr{K}^a y\rangle_2 \tag{5.7}$$

Hence, we have that for all $x \in L^2(\mathbb{R}_0^+)$ such that $\langle x_a, y\rangle_2 = 0$,

$$\langle x, (\rho(a) - \mathscr{K}^a)\, x\rangle_2 \geqslant [\rho(a) - \rho^{(1)}(a)]\, \|x\|_2^2 \tag{5.8}$$

Therefore, we are in the situation of Griffel[3] Proposition 10.31. Apply this proposition to get

$$\int_0^\infty du(u - \rho'(a))\, x_a(u)\, y_a(u) = \langle y_a, f_a\rangle_2 \leqslant \frac{1}{[\rho(a) - \rho^{(1)}(a)]}\, \|f_a\|_2^2 \tag{5.9}$$

Substitute (5.6) and use (5.3) to get

$$\rho''(a) \leqslant \frac{2}{[\rho(a) - \rho^{(1)}(a)]} \int_0^\infty du(u - \rho'(a))^2\, x_a^2(u) \tag{5.10}$$

Because of (4.14) and (5.11) below, the following two inequalities suffice for the upper bound in Theorem 3(c):

Lemma 5. $b^{*3} \int_0^\infty du(u - \rho'(a^*))^2\, x_{a^*}^2(u) = b^*(\frac{2}{3}a^* b^* - 1) \leqslant 0.72.$

Proof. See (4.2) and Theorems 3(a–b). ∎

Lemma 6. $-\rho^{(1)}(2.2) \in [3.3, 3.4]$.

Proof. See Section 5.2 below. ∎

5.2. Proof of Lemma 6: Spectral Analysis of $\mathscr{K}^{a^*}$

In this section we shall prove bounds for $\rho^{(1)}(2.2)$, using computer plots of $x_{a,\rho}$ for $a = 2.2$ and suitable values of ρ, Lemma 2 and the error estimates in Lemma 4. Lemma 3 guarantees that there are exactly as many zeros as seen in the plot.

In the same way as in (4.3) below, we have

$$\frac{d}{da}\rho^{(k)}(a) = \int_0^\infty du\, u x_a^{(k)}(u)^2 \geqslant 0 \tag{5.11}$$

where $x_a^{(k)}$ is the eigenfunction corresponding to the eigenvalue $\rho^{(k)}(a)$ (recall HHK Section 3.1). Hence, all the eigenvalues are increasing in a. Therefore we can take $a = 2.2$.

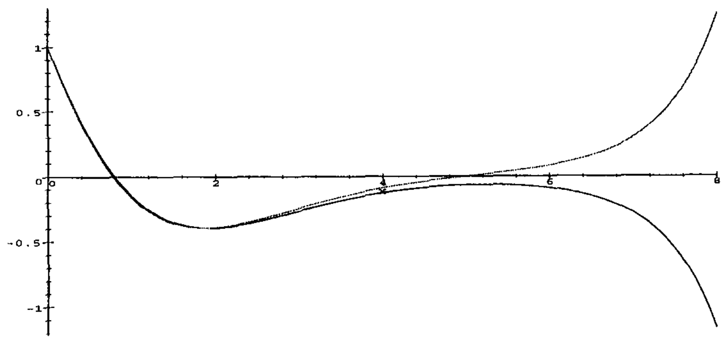

Fig. 3. The power series approximation of $x_{a,\rho}$ with $(a, \rho) = (2.2, -3.4)$, respectively, $(2.2, -3.3)$ and $k = 350$, $N = 8$.

By (2.8)

$$K(2, 2, \rho) \leqslant 2.15 \qquad \text{uniformly for} \quad \rho \in [-3.4, 0] \tag{5.12}$$

Again we pick $N = 8$ and $k = 350$. Then by (2.11),

$$C_k(2, 2, \rho) \leqslant 0.085 \qquad \text{uniformly for} \quad \rho \in [-3.4, 0] \tag{5.13}$$

Therefore, by (2.10), the difference between $x_{a,\rho}(u)$ and the power series approximation of $x_{a,\rho}(u)$ with 350 terms is smaller than or equal to 6×10^{-60}.

In Fig. 3 the sum of the first 350 terms of the power series of $x_{a,\rho}(u)$ is plotted for $a = 2.2$ and $\rho = -3.3$, respectively, $\rho = -3.4$. Since $c(2.2, -3.4) \leqslant N = 8$ and $c(2.2, -3.3) \leqslant N = 8$ (recall (2.4)), the number of zeros of $x_{2.2,-3.4}$ is 1 and the number of zeros of $x_{2.2,-3.3}$ is 2 by Lemma 3. This proves that $\rho^{(1)}(2.2) \in [-3.4, -3.3]$.

5.3. The Lower Bound for c^*

For some $s > 0$, let

$$y(u) = s(u - \rho'(a))\, x_a(u) \tag{5.14}$$

Then y is orthogonal to x_a (see (4.3)).

By (5.4)–(5.5) and Griffel[3] Proposition 10.31, it follows that

$$\tfrac{1}{2}\rho''(a) = \sup_{x : \langle x_a, x \rangle_2 = 0} \left[2\langle x, f_a \rangle_2 + \langle x, (\rho(a) - \mathscr{K}^a)\, x \rangle_2 \right] \tag{5.15}$$

(recall (5.6)). Substitution of $x = y$ (see (5.14)) gives

$$\frac{1}{2}\rho''(a) \geq \frac{2}{s}\|y\|_2^2 + \langle y, (\rho(a) - \mathscr{K}^a)\, y\rangle_2 \tag{5.16}$$

Next, compute for $a = a^*$,

$$\begin{aligned}(\mathscr{K}^{a^*}y)(u) &= s(u - \rho'(a^*))(\mathscr{K}^{a^*}x_{a^*})(u) + 4sux'_{a^*}(u) + 2sx_{a^*}(u)\\ &= s(4ux'_{a^*}(u) + 2x_{a^*}(u))\end{aligned}$$

where we use that $\rho(a^*) = 0$ (see (1.4)). Hence, by partial integration,

$$\begin{aligned}\langle y, \mathscr{K}^{a^*}y\rangle_2 &= s^2 \int_0^\infty 4u(u - \rho'(a^*))\, x'_{a^*}(u)\, x_{a^*}(u)\\ &= -2s^2\rho'(a^*)\end{aligned} \tag{5.18}$$

Furthermore, use (4.3) and (4.2) to compute

$$\begin{aligned}\|y\|_2^2 &= s^2\left(\int_0^\infty u^2x_{a^*}^2(u)\, du - \rho'(a^*)^2\right)\\ &= s^2\rho'(a)\,(\tfrac{2}{3}a^* - \rho'(a^*))\end{aligned} \tag{5.19}$$

Substituting (5.17)–(5.19) into (5.16) and maximizing over s, we get

$$\rho''(a^*) \geq \rho'(a^*)^3\,(\tfrac{2}{3}a^*b^* - 1)^2 \tag{5.20}$$

The lower bound now follows from the definition $c^{*2} = (\rho''(a^*)/\rho'(a^*)^3)$ (recall (1.4)) and Theorem 3(a–b)

Note. Just prior to completion of this paper, we received a letter from John Westwater explaining a different functional analytic method to obtain sharp numerical estimates on a^*, b^*, c^*. Rather than working with the Sturm–Liouville differential Eq. (2.1), he uses the variational problem in Westwater[8] and a truncation of the minimizer of this variational problem of an expansion into Laguerre polynomials. His method gives rigorous upper bounds on a^*. All other estimates are non-rigorous for lack of error estimates. The values found are fully in agreement with the bounds in Theorem 3(a–c).

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