THE CONSTANTS IN THE CLT

FOR THE EDWARDS MODEL

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Abstract

The Edwards model in one dimension is a transformed path measure for one-dimensional Brownian motion discouraging self-intersections. In van der Hofstad, den Hollander and König (preprint 1995) a central limit theorem (CLT) is proved for the fluctuations of the endpoint of the path around its linear asymptotics. In the present paper, we study the constants appearing in this CLT (which represent the mean and the variance) and the exponential rate of the normalizing constant. We prove that the variance is strictly smaller than 1, which shows that the weak interaction limit is singular. Furthermore, we give a relation between the normalizing constant in the Edwards model and the normalizing constant in the weakly interacting Domb-Joyce model. The Domb-Joyce model is the discrete analogue of the Edwards model based on simple random walk and is studied in van der Hofstad, den Hollander and König (preprint 1996).

The proofs are based on bounds for the eigenvalues of a certain one-parameter family of Sturm-Liouville differential operators. These bounds are obtained by using the monotonicity of the zeroes of the eigenfunctions in combination with computer plots of the power series approximation of the eigenfunctions and exact error estimates of the power series approximation.

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0 Motivation and main results

0.1 The Edwards model

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

$$\frac{d\widehat{P}_T^\beta}{d\widehat{P}} = \frac{1}{\widehat{Z}_T^\beta} \exp\left[-\beta \int_0^T ds \int_0^T dt \ \delta(B_s - B_t)\right] \qquad (T \geq 0). \tag{0.1}$$

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

$$\int_0^T ds \int_0^T dt \ \delta(B_s - B_t) = \int_{\mathbb{R}} dx \ L^2(T, x), \tag{0.2}$$

where $L(T, x)$ is the local time at x until time T. In [3] 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 $\mathcal{K}^a : L^2(\mathbb{R}_0^+) \cap C^2(\mathbb{R}_0^+) \to C(\mathbb{R}_0^+)$ by

$$\Big(\mathcal{K}^a x\Big)(u) = 2ux''(u) + 2x'(u) + (au - u^2)x(u) \qquad \text{for } u \in \mathbb{R}_0^+ = [0, \infty). \tag{0.3}$$

The Sturm-Liouville operator $\mathcal{K}^a$ will play a key role in the present paper.[1] It is symmetric and has a largest eigenvalue $\rho(a)$ with multiplicity 1. 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

$$\rho(a^*) = 0, \qquad b^* = \frac{1}{\rho'(a^*)}, \qquad c^{*2} = \frac{\rho''(a^*)}{\rho'(a^*)^3}. \tag{0.4}$$

[1]The operator $\mathcal{K}^a$ is a scaled version of the operator $\mathcal{L}^a$ originally analyzed in [2] Section 5, namely $(\mathcal{K}^a x)(u) = (\mathcal{L}^a \overline{x})(u/2)$ where $\overline{x}(u) = x(2u)$.

Theorem 1 *(van der Hofstad, den Hollander and König (preprint 1995)) For every* $\beta \in (0,\infty)$ *there exist* $b^*, c^* \in (0,\infty)$ *such that*

$$\lim_{T\to\infty} \widehat{P}_T^\beta\Big(\frac{|B_T| - b^*\beta^{\frac{1}{3}}T}{c^*\sqrt{T}} \le C\Big) = \mathcal{N}((-\infty, C]) \text{ for all } C \in \mathbb{R}, \tag{0.5}$$

where $\mathcal{N}$ *denotes the normal distribution with mean 0 and variance 1. Furthermore, there exists* $\widehat{L} \in (0,\infty)$ *such that*

$$\widehat{L} = \lim_{T\to\infty} e^{a^*\beta^{\frac{2}{3}}T}\widehat{Z}_T^\beta. \tag{0.6}$$

The simple dependence on β of the mean, the variance and the normalizing constant in Theorem 1 follows from Brownian scaling (see [3] Section 0.3).

Since the standard deviation c^* is *independent* of β, it is interesting to know whether c^* differs from 1. In Theorem 3(i-iii) below we shall give bounds on the constants a^*, b^* and c^*. Furthermore, Theorem 3(iv) relates the asymptotic behavior of the normalizing constant in the Edwards model, with the asymptotic behavior of the normalizing constant in the *Domb-Joyce model* that we shall introduce now.

0.2 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 w.r.t. the simple random walk measure. Let P_n^β be the measure on n-step paths given by

$$\frac{dP_n^\beta}{dP} = \frac{1}{Z_n^\beta}\exp\Big[-\beta\sum_{\substack{i,j=0\\ i\neq j}}^{n} 1_{\{S_i=S_j\}}\Big], \tag{0.7}$$

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 (0.1), where the Wiener measure is replaced by the simple random walk measure and the exponent in (0.1) by the exponent in (0.7). It is therefore the discrete analogue of the Edwards measure.

We have the following asymptotic behavior of Z_n^β, similar to (0.6):

Theorem 2 *(van der Hofstad, den Hollander and König (preprint 1996)) Let* $\beta_n \in (0, \infty)$ *be such that*

$$\beta_n \to 0 \text{ and } n^{\frac{3}{2}}\beta_n \to \infty \text{ as } n \to \infty. \tag{0.8}$$

Then there exists $L \in (0, \infty)$ *such that*

$$\lim_{n\to\infty} \beta_n^{-\frac{1}{3}} e^{r_n n} Z_n^{\beta_n} = L, \tag{0.9}$$

where r_n *satisfies*

$$\lim_{n\to\infty} \beta_n^{-\frac{2}{3}}\ r_n = a^*. \tag{0.10}$$

Theorem 2 is an important ingredient in the proof of the CLT for the weakly interacting Domb-Joyce model in [4]. This CLT fits nicely with the CLT for the Edwards model in Theorem 1, in the sense that the mean, the variance and the exponential rate of the normalizing constant have the same β_n-scaling if β_n satisfies (0.8). This is illustrated by (0.10) and (0.6). However, the behavior of the normalizing constant in (0.10) is structurally different from the one in (0.6), since there is no β-power in (refscalingnc).

0.3 Main theorem: Theorem 3

The following is our main theorem:

Theorem 3

- *(i)* $a^* \in [2.188, 2.189]$
- *(ii)* $b^* \in [1.104, 1.124]$
- *(iii)* $c^* \in [0.60, 0.66]$
- *(iv)* $\widehat{L} = \frac{a^*}{2} L > L.$

The proof of Theorem 3 is given in Sections 1-5 and is based on estimates of the eigenvalues of the differential operator $\mathcal{K}^a$ (recall (0.3)). Section 1 describes the Sturm-Liouville theory with which we can estimate the constants. In Sections 2-5 we derive the estimates for a^*,

b^*, c^*, $\widehat{L}$ and L respectively. These estimates are computer-assisted and we give exact error estimates.

The bounds in Theorem 3 (i-ii) can be made arbitrarily sharp by making the estimates of the eigenvalues sharper. For the bound in Theorem 3 (iii) this is not the case, which is due to the fact that c^* in (0.4) is a more complicated object.

0.4 Discussion

Our main results are that the constant c^*, giving the standard deviation of the polymer in both the Edwards model and the weakly interacting Domb-Joyce model, is strictly smaller than 1 and that the $\mathcal{O}(1)$-term of the normalizing constant in the CLT for the Edwards model is larger than the one in the CLT for the weakly interacting Domb-Joyce model.

The first statement means that the variances in the CLT's for the Domb-Joyce model and the Edwards model are discontinuous at $\beta = 0$ 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 $E(\frac{S_n^2}{n}) = \widehat{E}(\frac{B_T^2}{T}) = 1$ for all $n \in \mathbb{N}$ and $T > 0$. Note, on the other hand, that the mean of the CLT *is* continuous at $\beta = 0$.

The second statement means that the normalizing constant in the Edwards model is larger than the normalizing constant in the Domb-Joyce model. This is intuitively reasonable: simple random walk is restricted to the integers, while Brownian motion is free to move over the real line and can therefore optimize the partition function better.

1 Preparations: Lemmas 1-4

In this section we shall analyze the zeroes of the eigenfunctions of the Sturm-Liouville differential operator $\mathcal{K}^a$ (recall (0.3)). The method we use is more general and hence not restricted to $\mathcal{K}^a$.

1.1 Sturm-Liouville theory: Lemmas 1-3

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

$$\Big(\mathcal{K}^a x\Big)(u) = 2x''(u) + 2x'(u) + (au - u^2)x(u) = \rho x(u), \tag{1.1}$$

with

$$x_{a,\rho}(0) = 1, x'_{a,\rho}(0) = \rho \tag{1.2}$$

(see also [2] Section 2.6). This solution is unique by [2] Lemma 19, but by [2] 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 $\rho^{(k)}(a)$ (see [4] Section 3.1). In the sequel we shall use the extreme sensitivity of the tails of $x_{a,\rho}$ w.r.t. a and ρ to get sharp numerical estimates.

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 $u(a,\rho) < \infty$,*

$$\begin{aligned} \tfrac{\partial}{\partial\rho} u(a,\rho) &\geq 0, \\ \tfrac{\partial}{\partial a} u(a,\rho) &\leq 0. \end{aligned} \tag{1.3}$$

Proof. We shall prove the first statement only. The proof of the second statement is analogous.

Fix a and suppose $u(a,\rho) < \infty$ is a zero of $x_{a,\rho}$. Then, by the implicit function theorem and the fact that $x'_{a,\rho}(u(a,\rho)) \neq 0$, $\rho \mapsto u(a,\rho)$ is a differentiable function. By (1.17) below, $x_{a,\rho}$ can be represented as a power series with coefficients that are differentiable in a and ρ. Hence

$$y_{a,\rho}(u) = \frac{d}{d\rho} x_{a,\rho}(u) \tag{1.4}$$

exists. Differentiate $x_{a,\rho}(u(a,\rho)) = 0$ w.r.t. ρ to get

$$0 = x'_{a,\rho}(u(a,\rho)) \frac{\partial}{\partial\rho} u(a,\rho) + y_{a,\rho}(u(a,\rho)). \tag{1.5}$$

Thus, to prove Lemma 1 it is sufficient to prove that $x'_{a,\rho}(u(a,\rho))$ and $y_{a,\rho}(u(a,\rho))$ have opposite sign.

To that end, note that $y_{a,\rho}$ satisfies the inhomogeneous differential equation

$$\left(\mathcal{K}^a y_{a,\rho}\right)(u) - \rho y_{a,\rho}(u) = x_{a,\rho}(u), \tag{1.6}$$

with

$$y_{a,\rho}(0) = 0, y'_{a,\rho}(0) = 1, \tag{1.7}$$

which is obtained by differentiating (1.1-1.2) w.r.t. ρ. Now, let $u \mapsto \hat{x}_{a,\rho}(u)$ be any solution of (1.1-1.2) such that $\lim_{u\downarrow 0} \frac{\hat{x}_{a,\rho}(u)}{\ln u} = -1$ (see [2] (5.22)) and note that $x_{a,\rho}$ and $\hat{x}_{a,\rho}$ are a basis of solutions for the homogeneous equation $\mathcal{K}^a x = \rho x$. Since the Wronskian of the differential equation (1.1-1.2) equals

$$u x'_{a,\rho}(u)\hat{x}_{a,\rho}(u) - u x_{a,\rho}(u)\hat{x}'_{a,\rho}(u) \equiv 1, \tag{1.8}$$

the solution to (1.6-1.7) is given by

$$y_{a,\rho}(u) = -\hat{x}_{a,\rho}(u)\int_0^u \xi x^2_{a,\rho}(\xi)d\xi + x_{a,\rho}(u)\int_0^u \xi x_{a,\rho}(\xi)\hat{x}_{a,\rho}(\xi)d\xi. \tag{1.9}$$

Since $u = u(a,\rho)$ is a zero of $x_{a,\rho}$, we obtain

$$y_{a,\rho}(u(a,\rho)) = -\hat{x}_{a,\rho}(u(a,\rho))\int_0^{u(a,\rho)} \xi x^2_{a,\rho}(\xi)d\xi, \tag{1.10}$$

so $y_{a,\rho}(u(a,\rho))$ has opposite sign from $\hat{x}_{a,\rho}(u(a,\rho))$. Finally, substitution of $u = u(a,\rho)$ into (1.8) gives

$$u(a,\rho)x'_{a,\rho}(u(a,\rho))\hat{x}_{a,\rho}(u(a,\rho)) = 1, \tag{1.11}$$

which together with (1.10) proves that $x'_{a,\rho}(u(a,\rho))$ and $y_{a,\rho}(u(a,\rho))$ indeed have opposite sign. $\square$

Lemma 1 states that if there is a (finite) 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 zeroes to move to the negative axis. Hence, $x_{a,\rho}$ can only get more zeroes as ρ decreases or a increases.

Using Lemma 1, we shall prove the following stronger statement:

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

$$n(a,\rho) = \#\{\textit{finite zeroes of } x_{a,\rho}\}. \tag{1.12}$$

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 $\rho \in (\rho^{(k)}(a), \rho^{(k-1)}(a)] \quad (k \geq 1)$.

Proof. Fix $a \in \mathbb{R}$. For $k \in \mathbb{N}$, define

$$A_k = \{\rho : \exists I \subseteq \mathbb{R}_0^+ \text{ bounded such that } x_{a,\rho} \text{ has at least } k \text{ zeroes in } I\}. \tag{1.13}$$

Then A_k is an open interval, unbounded to the left by Lemma 1 and the fact that $x_{a,\rho}(0) = 1$. Consequently, A_k^c is a closed interval and has a smallest element $\overline{\rho}^{(k)}$. We shall show that $\overline{\rho}^{(k)} = \rho^{(k)}(a)$.

To that end, let $u_k(a,\rho)$ be the kth zero of $x_{a,\rho}$. Then

$$\lim_{\rho \uparrow \overline{\rho}^{(k)}} u_k(a,\rho) = \infty. \tag{1.14}$$

To see why, suppose that $\lim_{\rho \uparrow \overline{\rho}^{(k)}} u_k(a,\rho) = v < \infty$. By continuity of $\rho \mapsto x_{a,\rho}(u)$, $v = u_k(a, \overline{\rho}^{(k)})$ is the kth (finite) zero of $x_{a,\overline{\rho}^{(k)}}(u)$. Eq. (1.5), together with $x'_{a,\overline{\rho}^{(k)}}(v) \neq 0$ and $y_{a,\overline{\rho}^{(k)}}(v) \neq 0$ (recall (1.8-1.10)), give that $\frac{\partial}{\partial\rho} u_k(a, \overline{\rho}^{(k)}) > 0$, which is a contradiction.

Furthermore, since $\rho \mapsto x_{a,\rho}(u)$, $\rho \mapsto x'_{a,\rho}(u)$ and $\rho \mapsto x''_{a,\rho}(u)$ are continuous for all $u \in \mathbb{R}_0^+$ (see (1.17-1.18) below), $x_{a,\overline{\rho}^{(k)}}(u)$ and $x'_{a,\overline{\rho}^{(k)}}(u)$ have opposite sign for large u by the following reasoning. Let

$$c(a,\rho) = \frac{1}{2}a + \frac{1}{2}\sqrt{a^2 - 4\rho} \tag{1.15}$$

be the last zero of $f_{a,\rho}(u) = u^2 - au + \rho$. Take $\rho < \overline{\rho}^{(k)}$ such that $u_k(a,\rho) > c(a,\rho)$ (recall (1.14)). Then $x_{a,\rho}$ has a zero larger than $c(a,\rho)$. Next, rewrite (1.1) as

$$[u x'_{a,\rho}(u)]' = f_{a,\rho}(u) x_{a,\rho}(u), \tag{1.16}$$

where the $'$ stands for differentiation w.r.t. u. Then, for all $u \in [c(a,\rho), u_k(a,\rho))$, $x_{a,\rho}(u)$ and $x'_{a,\rho}(u)$ have opposite sign, since otherwise these signs would remain the same for all

$v \geq u$ by (1.16) and hence $x_{a,\rho}$ would not have a zero larger than u. (Note that $f_{a,\rho}(u) \geq 0$ for all $u \geq c(a,\rho)$.) Now let $\rho \uparrow \overline{\rho}^{(k)}$ and use (1.14) and the continuity of $c(a,\rho)$, to see that $x_{a,\overline{\rho}^{(k)}}(u)$ and $x'_{a,\overline{\rho}^{(k)}}(u)$ have opposite sign for $u > c(a,\overline{\rho}^{(k)})$. The only way this is possible is when $\lim_{u\to\infty} x_{a,\overline{\rho}^{(k)}}(u)$ exists and is bounded. Use [2] Lemma 20 to see that then $x_{a,\overline{\rho}^{(k)}}$ is in $L^2(\mathbb{R}_0^+)$. Hence, $\overline{\rho}^{(k)}$ has to be an eigenvalue of $\mathcal{K}^a$ in $L^2(\mathbb{R}_0^+)$. It is now easy to see that $\overline{\rho}^{(k)} = \rho^{(k)}(a)$ by counting the number of finite zeroes of $x_{a,\overline{\rho}^{(k)}}$, which has to be exactly $k-1$. $\square$

Lemma 3 *If $v \geq c(a,\rho)$ 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 $u \geq v$.*

Proof. Easy. See (1.16). $\square$

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

1.2 Power series approximation: Lemma 4

We end this preparatory section by explaining how we can determine the number of zeroes of $x_{a,\rho}$ in a bounded interval.

Use [2] (5.23) to write $x_{a,\rho}(u)$ as a power series

$$x_{a,\rho}(u) = \sum_{n=0}^{\infty} g_n u^n, \tag{1.17}$$

where the g_n's satisfy the recurrence relation

$$g_n = \frac{1}{2n^2}(\rho g_{n-1} - a g_{n-2} + g_{n-3}) \ (n \geq 1), \tag{1.18}$$

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

$$g_n \leq \frac{K(a,\rho)^n}{(n!)^{\frac{2}{3}}} \qquad (n \geq 1), \tag{1.19}$$

where $K(a,\rho)$ satisfies

$$\frac{|\rho|}{2^{\frac{5}{3}} K(a,\rho)} + \frac{|a|}{2^{\frac{4}{3}} K(a,\rho)^2} + \frac{1}{2K(a,\rho)^3} \leq 1. \tag{1.20}$$

In the sequel we shall take

$$K(a,\rho) = \max\Big\{2^{-\frac{2}{3}}|\rho|,\ \sqrt{\frac{3|a|}{2^{\frac{4}{3}}}},\ \sqrt[3]{3}\Big\}. \tag{1.21}$$

(This corresponds to bounding the first term in (1.20) 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 shall 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 (1.17).

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

$$|\sum_{n=k}^{\infty} g_n u^n| \leq \frac{[NC_k]^k}{(1-NC_k)\sqrt[3]{2\pi k}} \text{ uniformly for } u \in [0,N], \tag{1.22}$$

where C_k is given by

$$C_k = C_k(a,\rho) = \frac{K(a,\rho)e^{\frac{2}{3}}}{k^{\frac{2}{3}}}. \tag{1.23}$$

Proof. Use Stirling's inequality

$$n! \geq \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \tag{1.24}$$

and (1.19), to get

$$\begin{aligned} l.h.s.\ (1.22) &\leq \textstyle\sum_{n=k}^{\infty} \frac{[NC_n]^n}{\sqrt[3]{2\pi n}} \\ &= \textstyle\sum_{n=0}^{\infty} \frac{[NC_{n+k}]^{n+k}}{\sqrt[3]{2\pi(n+k)}} \\ &\leq \textstyle\frac{[NC_k]^k}{\sqrt[3]{2\pi k}} \sum_{n=0}^{\infty} [NC_k]^n. \end{aligned} \tag{1.25}$$

□

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

2 Proof of Theorem 3(i)

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 $a \leq a^*$. Next, (1.21) gives that

$$K(a, 0) \leq 1.7 \text{ uniformly for } a \leq 2.2. \tag{2.1}$$

Hence, in (1.23),

$$C_k \leq 0.07. \tag{2.2}$$

Thus, by (1.22), 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 Figure 1, Lemma 3 and the fact that $c(a, 0) = a < N = 8$ for $a \leq 2.2$ (recall (1.15)).

3 Proof of Theorem 3(ii)

3.1 The lower bound for b^*

First we derive an equality, (3.6) below, that we need later on to prove the lower bound for b^*.

For $a \in \mathbb{R}$ and $\beta \in \mathbb{R}^+$, define the 2-parameter family of differential operators $\mathcal{K}^{a,\beta}$: $L^2(\mathbb{R}_0^+) \cap C^2(\mathbb{R}_0^+) \mapsto C(\mathbb{R}_0^+)$ given by

$$\left(\mathcal{K}^{a,\beta} x\right)(u) = 2ux''(u) + 2x'(u) + (au - \beta u^2)x(u). \tag{3.1}$$

Let $\rho(a, \beta)$ be the largest eigenvalue of $\mathcal{K}^{a,\beta}$ in $L^2(\mathbb{R}_0^+)$. By a trivial scaling we get that for every $\beta \in \mathbb{R}^+$

$$\begin{gathered} \beta^{-\frac{1}{3}} \rho(a\beta^{\frac{2}{3}}, \beta) = \rho(a, 1) = \rho(a) \\ \text{with eigenfunction } x_{(a,\beta)} = \beta^{-\frac{1}{6}} x_{a\beta^{\frac{2}{3}}}(\cdot\beta^{-\frac{1}{3}}). \end{gathered} \tag{3.2}$$

Differentiation of (3.2) w.r.t. β on both sides gives

$$\frac{2}{3}a\beta^{-\frac{2}{3}}\rho_{(a)}(a\beta^{\frac{2}{3}},\beta)+\beta^{-\frac{1}{3}}\rho_{(\beta)}(a\beta^{\frac{2}{3}},\beta)-\frac{1}{3}\beta^{-\frac{4}{3}}\rho(a\beta^{\frac{2}{3}},\beta)=0, \tag{3.3}$$

where the subscript stands for differentiation w.r.t. that parameter. Next, use that $(a,\beta)\mapsto x_{(a,\beta)}$ is analytic as a function from $\mathbb{R}\times(0,\infty)$ to $L^2(\mathbb{R}_0^+)$ and that $||x_{(a,\beta)}||_{L^2(\mathbb{R}_0^+)}=1$, to get

$$\begin{aligned}\rho_{(\beta)}(a,\beta) &= \frac{\partial}{\partial\beta}\langle x_{(a,\beta)},\mathcal{K}^{a,\beta}x_{(a,\beta)}\rangle_{L^2(\mathbb{R}_0^+)} \\ &= -\int_0^\infty u^2 x^2_{(a,\beta)}(u)du,\end{aligned} \tag{3.4}$$

respectively,

$$\rho_{(a)}(a,\beta)=\int_0^\infty u x^2_{(a,\beta)}(u)du. \tag{3.5}$$

Substituting $a=a^*,\beta=1$, using (3.2) and (3.4-3.5) and $\rho(a^*)=0$, we get

$$\frac{2}{3}a^*\rho'(a^*)-\int_0^\infty du\ u^2\ x^2_{a^*}(u)=0. \tag{3.6}$$

To get the lower bound for b^*, use $\frac{1}{b^*}=\int_0^\infty du\ ux^2_{a^*}(u)$ and write out using partial integration:

$$\begin{aligned}a^*-\tfrac{2}{b^*} &= \textstyle\int_0^\infty du\ (a^*u-u^2)'x^2_{a^*}(u) \\ &= -2\textstyle\int_0^\infty du\ (a^*u-u^2)x_{a^*}(u)x'_{a^*}(u) \\ &= 4\textstyle\int_0^\infty du\ \ [x'_{a^*}(u)^2+ux''_{a^*}(u)x'_{a^*}(u)] \\ &= 2||x'||^2_{L^2(\mathbb{R}_0^+)}.\end{aligned} \tag{3.7}$$

Here the second equality uses (0.3), while the third equality again follows from partial integration. Therefore, a rough lower bound for b^* is

$$a^*-\frac{2}{b^*}\geq 0 \text{ or } b^*\geq\frac{2}{a^*}, \tag{3.8}$$

which together with Theorem 3(i) gives

$$b^* \geq 0.91. \tag{3.9}$$

However, (3.9) can be improved using (3.6), partial integration and the Cauchy-Schwarz inequality:

$$\begin{aligned} 1 &= -2\int_0^\infty du\ u x_{a^*}(u) x'_{a^*}(u) \\ &\leq 2\|x'\|_{L^2(\mathbb{R}_0^+)} \sqrt{\int_0^\infty du\ u^2 x_{a^*}^2(u)} \\ &= \sqrt{2}\|x'\|_{L^2(\mathbb{R}_0^+)} \sqrt{\tfrac{4}{3}\tfrac{a^*}{b^*}} \\ &= \tfrac{1}{b^*}\sqrt{a^*b^* - 2}\sqrt{\tfrac{4}{3}a^*}. \end{aligned} \tag{3.10}$$

Rewrite this to get

$$a^*b^* - 2 \geq b^{*2}\frac{3}{4}\frac{1}{a^*} \tag{3.11}$$

or

$$b^* \geq \frac{2}{a^*} + b^{*2}\frac{3}{4}\frac{1}{a^{*2}}. \tag{3.12}$$

Now, insert (3.9) into the r.h.s. of (3.12) and use Theorem 3(i) to get

$$b^* \geq 1.043. \tag{3.13}$$

Iterating (3.12) seven times, each time with the improved lower bound in the r.h.s., we arrive at the lower bound in Theorem 3(ii).

3.2 The upper bound for b^*

To prove the upper bound for b^*, use the monotonicity of $a \mapsto \rho'(a)$ and the relation $b^* = [\rho'(a^*)]^{-1}$ (see [2] Theorems 5-6 and Theorem 3(i)) to get that

$$b^* \leq \frac{1}{100[\rho(2.188) - \rho(2.178)]}. \tag{3.14}$$

Furthermore, $c(a,\rho) \le 3 < N = 8$ for these values of a, ρ (recall (1.15)), so that Lemma 3 applies. Recall (1.21) to get

$$K(a,\rho) \le 1.7 \text{ uniformly for } \rho \in [-0.0096, 0], a \in [2.178, 2.188]. \tag{3.15}$$

Hence (1.23) gives

$$C_k(a,\rho) \le 0.07 \text{ uniformly for } \rho \in [-0.0096, 0], a \in [2.178, 2.188]. \tag{3.16}$$

Thus, by (1.22), 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^{-89} (for these values of N, a, ρ and k). Now use Lemma 2 and Figure 2 to get that

$$\begin{aligned} \rho(2.178) &\le -0.0096 \\ \rho(2.188) &\ge -0.0007, \end{aligned} \tag{3.17}$$

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 $(a,\rho) = (2.187, -0, 0007)$).

4 Proof of Theorem 3(iii)

In Sections 4.1-4.2 we prove the upper bound for c^*, in Section 4.3 the lower bound for c^*.

4.1 The upper bound for c^*: Lemmas 5-6

By differentiating (3.5) w.r.t. a (take $\beta = 1$ and use (3.2)), we get

$$\rho''(a) = 2 \int_0^\infty du \; u x_a(u) y_a(u), \tag{4.1}$$

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

$$y_a(u) = \frac{d}{da} x_a(u). \tag{4.2}$$

Differentiating the relation $||x_a||^2_{L^2(\mathbb{R}_0^+)} = 1$ w.r.t. a, we get

$$\langle x_a, y_a \rangle_{L^2(\mathbb{R}_0^+)} = 0. \tag{4.3}$$

Hence, we can rewrite (4.1) as

$$\rho''(a) = 2 \int_0^\infty du\ (u - \rho'(a)) x_a(u)\ y_a(u). \tag{4.4}$$

Note that by (3.2) and (3.5) also $u \mapsto (u - \rho'(a))x_a(u)$ is orthogonal to x_a (again take $\beta = 1$). Furthermore, differentiating the eigenvalue relation $\mathcal{K}^a x_a = \rho(a) x_a$ w.r.t. a, we get that y_a satisfies the inhomogeneous differential equation

$$-\Big(\mathcal{K}^a y\Big)(u) + \rho(a) y(u) = f_a(u), \tag{4.5}$$

where

$$f_a(u) = (u - \rho'(a)) x_a(u). \tag{4.6}$$

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

$$\rho^{(1)}(a) = \sup_{y:||y||_{L^2}=1, \langle x_a, y\rangle_{L^2}=0} \langle y, \mathcal{K}^a y \rangle_{L^2}. \tag{4.7}$$

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

$$\langle x, (\rho(a) - \mathcal{K}^a)\, x \rangle_{L^2} \geq [\rho(a) - \rho^{(1)}(a)] ||x||^2_{L^2(\mathbb{R}_0^+)}. \tag{4.8}$$

Therefore, we are in the situation of Griffel (1988) Proposition 10.31. Apply this proposition to get

$$\langle y, f_a \rangle_{L^2} \leq \frac{1}{[\rho(a) - \rho^{(1)}(a)]} ||f_a||^2_{L^2}. \tag{4.9}$$

Substitute (4.6) and use (4.3) to get

$$\rho''(a) \leq \frac{2}{[\rho(a) - \rho^{(1)}(a)]} \int_0^\infty du\ (u - \rho'(a))^2\ x_a^2(u). \tag{4.10}$$

Because of (3.17) and (4.11) below, the following two inequalities suffice for the upper bound in Theorem 3(iii):

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

Proof. See (3.6) and Theorems 3(i-ii). □

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

Proof. See Section 4.2 below. □

4.2 Proof of Lemma 6: Spectral analysis of $\mathcal{K}^{a^*}$

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 zeroes as seen in the plot.

In the same way as in (3.4-3.5) below, we have

$$\frac{d}{da}\rho^{(k)}(a) = \int_0^\infty du\ u x_a^{(k)}(u)^2 \geq 0, \tag{4.11}$$

where $x_a^{(k)}$ is the eigenfunction corresponding to the eigenvalue $\rho^{(k)}(a)$ (recall [4] Section 3.1). Hence, all the eigenvalues are increasing in a. Therefore we can take $a = 2.2$. By (1.20)

$$K(2.2, \rho) \leq 2.15 \text{ uniformly for } \rho \in [-3.4, 0]. \tag{4.12}$$

Again we pick $N = 8$ and $k = 350$. Then by (1.23),

$$C_k(2.2, \rho) \leq 0.085 \text{ uniformly for } \rho \in [-3.4, 0]. \tag{4.13}$$

Therefore, by (1.22), 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 Figure 3 the sum of the first 350 terms of the powerseries of $x_{a,\rho}(u)$ is plotted for $a = 2.2$ and $\rho = -3.3$, respectively, $\rho = -3.4$. Since $c(2.2, -3.4) \leq 8$ and $c(2.2, -3.3) \leq 8$ (recall (1.15)), the number of zeroes of $x_{2.2,-3.4}$ is 1 and the number of zeroes of $x_{2.2,-3.3}$ is 2 by Lemma 3. This proves that $\rho^{(1)}(2.2) \in [-3.4, -3.3]$.

4.3 The lower bound for c^*

For some $s > 0$, let

$$y(u) = s(u - \rho'(a))x_a(u). \tag{4.14}$$

Then y is orthogonal to x_a (see (3.2) and (3.5) with $\beta = 1$). By (4.5) and Griffel (1988) Proposition 10.31, it follows that

$$\frac{1}{2}\rho''(a) = \sup_{x:\langle x_a, x\rangle_{L^2}=0} [2\langle x, f_a\rangle_{L^2} + \langle x, (\rho(a) - \mathcal{K}^a)\, x\rangle_{L^2}] \tag{4.15}$$

(recall (4.6)). Substitution of $x = y$ (see (4.14)) gives

$$\frac{1}{2}\rho''(a) \geq \frac{2}{s}\|y\|^2_{L^2} + \langle y, (\rho(a) - \mathcal{K}^a)\, y\rangle_{L^2}. \tag{4.16}$$

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

$$\begin{aligned} (\mathcal{K}^{a^*}y)(u) &= s(u - \rho'(a^*))(\mathcal{K}^{a^*}x_{a^*})(u) + 4sux'_{a^*}(u) + 2sx_{a^*}(u) \\ &= s(4ux'_{a^*}(u) + 2x_{a^*}(u)), \end{aligned} \tag{4.17}$$

where we use that $\rho(a^*) = 0$ (see (0.4)). Hence

$$\begin{aligned} \langle y, \mathcal{K}^{a^*}y\rangle_{L^2} &= s^2 \textstyle\int_0^\infty 4u(u - \rho'(a^*))x'_{a^*}(u)x_{a^*}(u) \\ &= -2s^2\rho'(a^*). \end{aligned} \tag{4.18}$$

Furthermore, use (3.5) for $\beta = 1$ and (3.6) to compute

$$\begin{aligned} \|y\|^2_{L^2} &= s^2 \left(\textstyle\int_0^\infty u^2x^2_{a^*}(u)du - \rho'(a^*)^2\right) \\ &= s^2\rho'(a^*)(\tfrac{2}{3}a^* - \rho'(a^*)). \end{aligned} \tag{4.19}$$

Substituting (4.17-4.19) into (4.16) and maximizing over s, we get

$$\rho''(a^*) \geq \rho'(a^*)^3 \left(\frac{2}{3}a^*b^* - 1\right)^2. \tag{4.20}$$

The lower bound now follows from the definition $c^{*2} = \frac{\rho''(a^*)}{\rho'(a^*)^3}$ (recall (0.4)) and Theorem 3(i-ii).

5 Proof of Theorem 3(iv)

Recall [3] Proposition 1 and [4] Proposition 1 where $\widehat{L}$ and L appear. In this section we use the representations of $\widehat{L}$ and L to prove that $\widehat{L} = \frac{a^*}{2}L$. Since $a^* > 2$ by Theorem 3 (i), this will prove that $\widehat{L} > L$ as claimed.

Recall from [3] (2.33) and Lemmas 5-7, and [4] (3.19) and (2.34-2.35) that

$$\begin{aligned} \widehat{L} &= b^* \langle x_{a^*}, z_{a^*} \rangle_{L^2} \langle x_{a^*}, z_{a^*} \rangle^{\circ}_{L^2} && (5.1) \\ L &= \frac{b^*}{2} \langle x_{a^*}, z_{a^*} \rangle^2_{L^2}, && (5.2) \end{aligned}$$

(see footnote 1 for the factor $\frac{1}{2}$) where z_{a^*} satisfies the Airy equation

$$2z''(u) + (a^* - u)z(u) = 0 \qquad (u \in \mathbb{R}). \tag{5.3}$$

Hence we have to prove that

$$\langle x_{a^*}, z_{a^*} \rangle^{\circ}_{L^2} = \frac{a^*}{2} \langle x_{a^*}, z_{a^*} \rangle_{L^2}. \tag{5.4}$$

The proof relies on the fact that the differential equations for x_{a^*} (recall (0.3)), respectively, z_{a^*} (recall (5.3)) are similar.

Since $\mathcal{K}^{a^*} x_{a^*} = \rho(a^*) x_{a^*} = 0$ (recall (0.4)) and $\mathcal{K}^{a^*}$ is symmetric in $L^2(\mathbb{R}_0^+)$, we have

$$0 = \langle (\mathcal{K}^{a^*})^i x_{a^*}, z_{a^*} \rangle_{L^2} = \langle x_{a^*}, (\mathcal{K}^{a^*})^i z_{a^*} \rangle_{L^2} \qquad (i = 1, 2). \tag{5.5}$$

Compute (for $i = 1$)

$$\left(\mathcal{K}^{a^*} z_{a^*}\right)(u) = 2z'_{a^*}(u) + u\left[2z''_{a^*}(u) + (a^* - u)z_{a^*}(u)\right] = 2z'_{a^*}(u). \tag{5.6}$$

This gives (for $i = 2$)

$$\begin{aligned} \left((\mathcal{K}^{a^*})^2 z_{a^*}\right)(u) &= 2\left(\mathcal{K}^{a^*} z'_{a^*}\right)(u) \\ &= 4z''_{a^*}(u) + 2u\left[2z'''_{a^*}(u) + (a^* - u)z'_{a^*}(u)\right] && (5.7) \\ &= 4z''_{a^*}(u) + 2u z_{a^*}(u). \end{aligned}$$

Substitution of (5.3) into (5.7) gives

$$\left((\mathcal{K}^{a^*})^2 z_{a^*}\right)(u) = (4u - 2a^*) z_{a^*}(u). \tag{5.8}$$

After substituting (5.8) into (5.5) for $i = 2$, we end up with (5.4).

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 equation (1.1), he uses the variational problem in Westwater (1984) 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 (i-iii).

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Figure caption

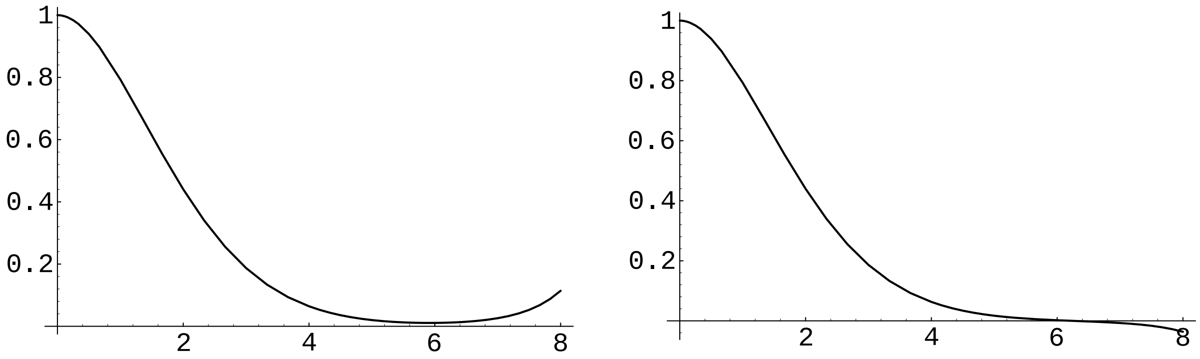

Figure 1a-b: The power series approximation of $x_{a,0}$ with $a = 2.187$, respectively, $a = 2.188$ and $N = 8, k = 350$.

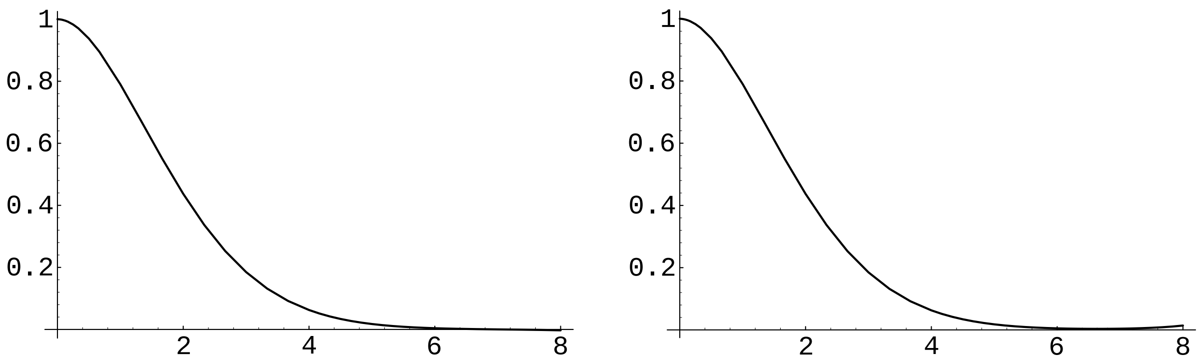

Figure 2a-b: The power series approximation of $x_{a,\rho}$ with $(a, \rho) = (2.187, -0.0096)$, respectively, $(a, \rho) = (2.177, -0.0007)$ and $N = 8, k = 350$.

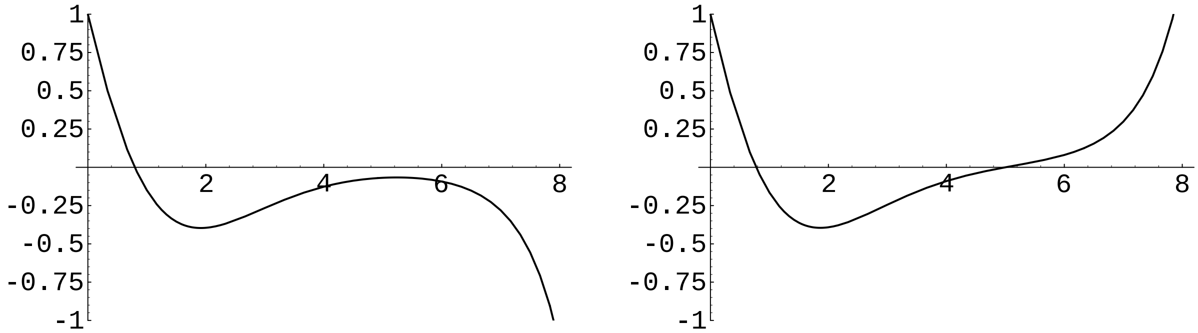

Figure 3a-b: The power series approximation of $x_{a,\rho}$ with $(a,\rho) = (2.2, -3.4)$, respectively, $(2.2, -3.3)$ and $k = 350, N = 8$.