HIGHER ENERGY STATE APPROXIMATIONS IN THE 'MANY INTERACTING WORLDS' MODEL

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ABSTRACT. In the 'Many Interacting Worlds' (MIW) discrete Hamiltonian system approximation of Schrödinger's wave equation, introduced in [11], convergence of ground states to the Normal ground state of the quantum harmonic oscillator, via Stein's method, in Wasserstein-1 distance with rate $\mathcal{O}(\sqrt{\log N}/N)$ has been shown [13], [5], [15]. In this context, we construct approximate higher energy states of the MIW system, and show their convergence with the same rate in Wasserstein-1 distance to higher energy states of the quantum harmonic oscillator. In terms of techniques, we apply the 'differential equation' approach to Stein's method, which allows to handle behavior near zeros of the higher energy states.

1. INTRODUCTION

Consider the recent 'Many Interacting Worlds' (MIW) discrete Hamiltonian system approximation [11] of the Schrödinger equation

$$i\hbar\partial_t\psi(t,x) = -\frac{\hbar^2}{2m}\partial_{xx}\psi(t,x) + x^2\psi(t,x), \tag{1.1}$$

governing the wave function in a one dimensional quantum mechanical system. Namely, following de Broglie-Bohm's interpretation [1] of (1.1), write $\psi = \sqrt{P}e^{iS/\hbar}$ in terms of a probability density P of the location of a particle and its momentum $\partial_x S$, where

$$\partial_t P + \partial_x\big(P(\partial_x S)\big) = 0, \tag{1.2}$$

$$\partial_t S + \frac{1}{2m}(\partial_x S)^2 + x^2 - \frac{\hbar^2}{4m}\Big(\partial_{xx}P/P - \frac{1}{2}\big(\partial_x P/P\big)^2\Big) = 0.$$

As discussed in [1], one may interpret (1.2) via a Hamiltonian system where the average energy

$$\bar{H} = \int P(x)\left(\frac{1}{2m}(\partial_x S)^2 + x^2 + \frac{\hbar^2}{8m}\left(\frac{\partial_x P}{P}\right)^2\right)\,dx. \tag{1.3}$$

In the MIW approach [11], a discretized Hamiltonian

$$\bar{H}_{\mathrm{MIW}} = \sum_{n=1}^{N}\frac{1}{2m}p_n^2 + \sum_{n=1}^{N}x_n^2 + \sum_{n=1}^{N}\frac{\hbar^2}{8m}\left(\frac{\partial_x P(x_n)}{P(x_n)}\right)^2$$

is formulated where $(x_n)_{n=1}^N$, with boundary conditions $x_0 = -\infty$ and $x_{N+1} = \infty$, are the locations of N 'world' particles, and $(p_n)_{n=1}^N$ are their momenta. Therefore, the average energy $\frac{1}{N}\bar{H}_{\mathrm{MIW}}$ formally approximates $\bar{H}$. We remark that $U(x_n) = \big(\partial_x P(x_n)/P(x_n)\big)^2$ represents a discretized form of Bohm's 'quantum mechanical' potential in reference to a 'classical' $V(x_n) = x_n^2$ potential.

In [11], the sequence $(x_n)_{n=1}^N$ is taken according to the mass $1/(N+1)$ quantiles of P, that is when $\int_{x_n}^{x_{n+1}} P(u)\,du = 1/(N+1)$ for $0 \leq n \leq N$. For large N, assuming that P is smooth, the gaps $x_{n+1} - x_n$ should vanish, and so $P(x_n) \approx \frac{1}{(N+1)(x_{n+1}-x_n)}$.
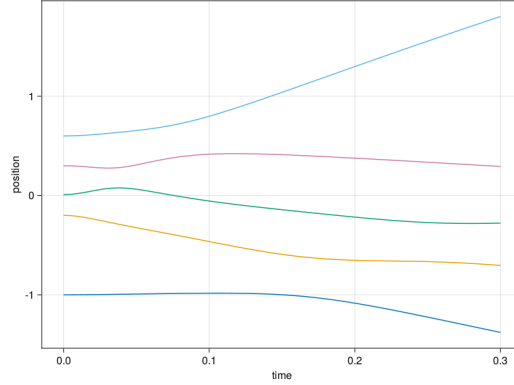
FIGURE 1. A simulation of MIW $N = 5$ dynamics.

Moreover, the derivative $\partial_x P(x_n) \approx \frac{P(x_{n+1}) - P(x_n)}{x_{n+1} - x_n}$. Therefore,

$$\frac{\partial_x P(x_n)}{P(x_n)} \approx (N+1)\partial_x P(x_n)(x_{n+1} - x_n)$$

$$\approx (N+1)(P(x_{n+1}) - P(x_n)) \approx \frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}}. \tag{1.4}$$

Note that interestingly the scale parameter N cancels here.

Putting this approximation into $U(t, x_n)$, and choosing units so that each 'world' particle has unit mass, and so that $\hbar^2 = 8m$, we will work with the discrete Hamiltonian

$$H_{\mathrm{MIW}} = \sum_{n=1}^{N} \frac{1}{2}p_n^2 + \sum_{n=1}^{N} x_n^2 + \sum_{n=1}^{N} \left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}} \right)^2, \tag{1.5}$$

through which the time evolution of the MIW system $(x_n = x_n(t))_{n=1}^{N}$, $(p_n = p_n(t))_{n=1}^{N}$, with $x_0 = -\infty$, $x_{N+1} = \infty$ and $N \geq 2$, is given by

$$p_n = \frac{dx_n}{dt} = \frac{\partial}{\partial p_n} H_{\mathrm{MIW}} \quad \text{and} \quad \frac{dp_n}{dt} = -\frac{\partial}{\partial x_n} H_{\mathrm{MIW}}. \tag{1.6}$$

We will say that a stationary configuration $(x_n)_{n=1}^{N}$ is one in which $p_n = \frac{dx_n}{dt} = \frac{dp_n}{dt} = 0$ for all $1 \leq n \leq N$.

Figure 1 shows the numerical simulation of the nonstationary dynamics of a five particle system starting at the given initial positions, and $x_0 = -\infty$ and $x_6 = \infty$.

We comment that other discretizations of U, involving more involved Taylor expansions, have been considered in [9]. We also mention higher dimensional MIW dynamics have been considered in works [12], [15], [18]. However, in the following, we will focus on the one dimensional formulation given above as it will allow some mathematical analysis.

1.1. **General aims.** Perhaps the main question at this point is whether indeed the discrete evolution with respect to Hamiltonian (1.5) approximates the continuous one in terms of (1.3). In this generality, this is an open question.

However, previous work has considered certain 'ground state' approximations. A ground state configuration $(x_n)_{n=1}^{N}$ is an increasing sequence on which H_{MIW} is minimized. In such a state, the system is stationary: $p_n = \partial_t x_n = 0$ for $1 \leq n \leq N$. In this time-independent setting, we observe

$$H_{\mathrm{MIW}} = H = \sum_{n=1}^{N} x_n^2 + \sum_{n=1}^{N} \left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}} \right)^2. \tag{1.7}$$

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Following [11], consider $A = \sum_{n=2}^{N}(x_{n-1} - x_n)\frac{1}{x_n - x_{n-1}} = -(N-1)$. Summation by parts, noting $x_0 = -\infty$, $x_{N+1} = \infty$ and $N \geq 2$, together with the Cauchy-Schwartz inequality, yields

$$\frac{A^2}{\sum_{n=1}^{N} x_n^2} \leq \sum_{n=1}^{N}\left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}}\right)^2, \tag{1.8}$$

with equality if and only if there is a constant c such that, for all $1 \leq n \leq N$,

$$-x_n = c\left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}}\right). \tag{1.9}$$

Hence, $H \geq V + A^2/V$, where $V = \sum_{n=1}^{N} x_n^2$. Optimizing over V, we get that $H \geq 2|A| = 2(N-1)$, with equality exactly when (1.9) holds and $V = N - 1$. Moreover, in this case, by summing the squares of both sides of (1.9), we have $V = c^2 \sum_{n=1}^{N}\left(\frac{1}{x_{n+1}-x_n} - \frac{1}{x_n - x_{n-1}}\right)^2 = c^2 \frac{A^2}{V}$, and so $c^2 = 1$, as $V = |A| = N - 1$. Since the sign of c determines only whether the order of $(x_n)_{n=1}^{N}$ is reversed, one may choose $c = 1$.

In particular, the corresponding sequence $(x_n)_{n=1}^{N}$ satisfying

$$\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}} = -x_n,$$

with boundary conditions $\frac{1}{x_2 - x_1} = -x_1$ and $\frac{1}{x_N - x_{N-1}} = x_N$, as $x_0 = -\infty$ and $x_{N+1} = \infty$, is the unique increasing minimum of H, and is therefore a ground state. Although the sequence values $x_n = x_n^{(N)}$ depend on N, to simplify notation, we will suppress the superscript in the following.

A question was posed in [11] whether the empirical distribution of these ground states $(x_n)_{n=1}^{N}$ converged as $N \uparrow \infty$ to the standard Normal distribution, that is the ground state of the time-homogeneous Schrödinger's equation, namely that of the quantum harmonic oscillator. This was recently resolved in the affirmative in [13, 5]; see also [15].

Indeed, we were inspired by the convergence shown there in Wasserstein-1 distance, with upper and lower rates of order $\frac{\sqrt{\log N}}{N}$, in [13, 5], via a form of Stein's method (cf. surveys [2], [16]).

1.2. Informal statement of results.

In this context, the goal of this paper is to study certain approximations of higher energy critical sequences of H in (1.7), and to investigate their convergence in Wasserstein-1 distance to higher energy states of the continuous quantum harmonic oscillator system. After the Normal ground state, the next continuous energy state of the quantum harmonic oscillator is the Maxwellian distribution. Higher continuous energy states, described later, can be defined in terms of the Hermite polynomials.

We comment that in [14], empirical distributions of sequences, seen as ground states of related systems but with different quantum potentials U, were shown to converge in Wasserstein-1 distance to the Maxwellian; see also [6] which considers ground state sequences for systems with 'Coulomb' potential V and an associated quantum potential U. However, as remarked in [14], to show validity of the MIW model, one would like to show such convergences with respect to 'critical' sequences corresponding to critical points of H to the Maxwellian and other higher energy continuum states. A difficulty is that it does not seem so facile to analyze the exact critical points of H, where $\nabla H = 0$, other than that corresponding to the global minimum. Our work in this respect will be to consider certain 'approximations' of these critical points.

Informally, our results include the following:

(a) In Theorem 2.1, we show existence and uniqueness of specific potential approximations of critical points, which we will call MIW sequences.
(b) The 'no-gap' property and spanning order of the MIW sequence, that is that $x_{n+1} - x_n$ vanishes and $x_1, x_N = \mathcal{O}(\sqrt{\log N})$ as $N \uparrow \infty$, is given in Theorem 2.3.
(c) We show in Theorem 2.4, via a form of Stein's method, that the empirical distributions of these sequences converge in Wasserstein-1 distance with rate $O(\sqrt{\log N}/N)$ to the Maxwellian and the other higher energy continuum state distributions.

(d) Finally, in Theorem 2.5, we show that the gradient of H on these sequences vanishes in a sense pointwise as $N \uparrow \infty$, and therefore these sequences may be viewed as approximate 'critical' points of H.

1.3. **MIW sequences and higher energy functions.** The sequences we consider are of the following type. Let f be a smooth, nonnegative function on $\mathbb{R}$. We will say an MIW sequence of f is a strictly increasing sequence $(x_n)_{n=1}^N$ on $\mathbb{R}$, away from the zeroes of f, satisfying the relation

$$\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}} = \frac{f'(x_n)}{f(x_n)} \tag{1.10}$$

for $1 < n < N$. The rationale for such a formulation is that (1.10) is a type of 'quantile' approximation, similar to (1.4), where $P'(x_n)/P(x_n)$ is replaced by $f'(x_n)/f(x_n)$. Note that we have chosen $(x_n)_{n=1}^N$ as increasing, although an alternate definition where the sequence is decreasing could also be used as in [13].

We will say that an MIW sequence $(x_n)_{n=1}^N$, contained in a possibly infinite interval (a, b), satisfies the 'left' and 'right' boundary conditions at $x_0 = a$ and $x_{N+1} = b$ if $\frac{1}{x_2 - x_1} - \frac{1}{x_1 - a} = \frac{f'(x_1)}{f(x_1)}$ and $\frac{1}{b - x_N} - \frac{1}{x_N - x_{N-1}} = \frac{f'(x_N)}{f(x_N)}$, respectively hold and are well defined. Note in the case $N = 1$ that the sequence (x_1) is well-defined exactly when one or both of a, b is finite. With a right boundary condition of $b = \infty$, by summing (1.10) over n and taking the reciprocal, the MIW sequence satisfies

$$x_{n+1} = x_n - \left(\sum_{k=n+1}^N \frac{f'(x_k)}{f(x_k)} \right)^{-1}, \tag{1.11}$$

for $1 \le n < N$. In this generality, it is not clear that such MIW sequences exist or are unique, even when f is strictly positive! See Appendix B for some counter-examples.

However, in this article, we will be concerned with stable states f of the quantum harmonic oscillator, for which we show MIW sequences may be constructed. For $\ell \ge 0$, we define the functions

$$f(x) = c p_\ell(x)^2 e^{-\frac{1}{2}x^2} \tag{1.12}$$

as higher energy functions, where $c \in \mathbb{R}^+$ is a normalization to make f a probability density. Here, p_ℓ is the ℓth Hermite polynomial, $p_\ell(x) = (-1)^\ell e^{\frac{1}{2}x^2} \frac{d^\ell}{dx^\ell} e^{-\frac{1}{2}x^2}$. Alternatively, the Hermite polynomials may be specified in terms of the differential equation $p_\ell''(x) = x p_\ell'(x) - \ell p_\ell(x)$.

We say the order of $f(x)$ is the order of $p_\ell(x)$, namely $\ell \ge 0$. Note that $p_0 = 1$, in which case $f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$ is the standard normal density. As well, $p_1 = x^2$, in which case $f(x) = \sqrt{\frac{8}{\pi}} x^2 e^{-\frac{1}{2}x^2}$ is the Maxwellian distribution density. We observe that the ℓth order higher energy function f has exactly ℓ roots (Lemma A.1), and is symmetric and log-concave (Lemma A.2).

1.4. **Proof ideas for the main theorems.** Our method of constructing MIW sequences with respect to ℓth order higher energy function f in the proof of Theorem 2.1 will be to create subsequences that lie entirely within the $\ell + 1$ regions of strict positivity of f. These subsequences, with specified numbers of points in each region, will be created so that their boundary conditions allow them to be strung together to form the desired MIW sequence.

The strategy of this construction follows partly the path taken in [13] with respect to the Normal density (the order zero strictly positive higher energy function), although there are new difficulties and differences, since higher energy functions of order $\ell \ge 1$ have ℓ roots to be bridged. We will define functions $(\chi_n(x))_{n \ge 1}$ inductively on appropriate domains in the $\ell + 1$ regions of strict positivity of f, where $\chi_1(x) = x$, and

$$\frac{1}{\chi_{n+1}(x) - \chi_n(x)} - \frac{1}{\chi_n(x) - \chi_{n-1}(x)} = \frac{f'(\chi_n(x))}{f(\chi_n(x))},$$

so that by adjusting the value x, the sequence $(\chi_n(x))_{n=1}^N$ will be an MIW sequence with appropriate left and right boundary conditions $\chi_0(x)$ and $\chi_{N+1}(x)$. We derive uniqueness of the MIW sequence,

with prescribed numbers of points in each region of strict positivity of f, via this construction, as sequences with different initial values, which determine the other points, must satisfy different boundary conditions.

An ingredient for the proofs of the Wasserstein-1 convergence and stability in Theorems 2.4 and 2.5, as well as intrinsic interest, will be to describe in Theorem 2.3 that the constructed MIW sequences have a 'no gap' property in that the maximal gap between points x_n and x_{n+1} for $1 \leq n \leq N-1$ vanishes as $N \uparrow \infty$. This will be a consequence of the MIW recursion that $(x_n)_{n=1}^N$ satisfies, and that gaps near the roots and at extremities, which we show are the largest, vanish as the number of points in the strictly positive intervals diverge as $N \uparrow \infty$. We will also specify $O\big(\sqrt{\log N}\big)$ asymptotics of x_1, x_N as $N \uparrow \infty$, generalizing estimates in [5] in the case of Normal density.

Proofs of convergence in Wasserstein-1 distance, with bounding rate of $\mathcal{O}\big(\sqrt{\log N}/N\big)$, of the empirical measures of the MIW sequences constructed in Theorem 2.4 to distributions with higher energy densities f follow the general Stein's differential equation approach [3], [4], [17] as opposed to methods involving zero-bias distributions (cf. [10]) as in [13, 5] with respect to the Normal density, and [14] with respect to the Maxwellian density. See also [15][Example 3.7] where a form of the differential Stein equation approach, fashioned to estimate directly between the empirical measure and the higher energy distribution, was used to show similar convergence with respect to the Normal density. We mention [15][Theorem 3.4] contains abstract Wasserstein-1 distance bounds in this vein between empirical measures of symmetric monotone sequences and distributions with density proportional to $b(x)e^{-\frac{1}{2}x^2}$ where b is nonnegative with $b(x) > 0$ for $x \neq 0$, although these do not apply in our general context.

A main difficulty to surmount is that the higher energy densities of order $\ell \geq 1$ have roots where singularities arise in the method. In this respect, we employ an 'intermediate' continuous distribution as in [13, 5] to bound the distance between it and the empirical measure. We then apply a suitable form of the differential equation approach to bound the distance between the 'intermediate' and higher energy distributions. This requires a detailed analysis of Stein method bounding terms, near zeros of f and at $\pm\infty$, that we provide.

Our tack, as in the existence and uniqueness arguments, is to separate $\mathbb{R}$ into intervals of strict positivity, bounded by the zeros of f, and to bound Wasserstein-1 distances between empirical distributions and distributions with density proportional to f restricted to each interval. We obtain bounds in terms of of order $(x_N - x_1)/N$ where x_1, x_N are the first and last points in the interval. When put together, we obtain the desired rate of convergence in Wasserstein-1 distance of the whole sequence on $\mathbb{R}$.

Finally, by explicit computation of the gradient of H on MIW sequences, we will show in the proof of Theorem 2.5 that, for every point t away from zeros of f, the partial derivative of H with respect to the closest point x_n in the MIW sequence constructed converges to $\big(t^2 - (f'(t)/f(t))^2 - 2[f'(t)/f(t)]'\big)'$ as $N \to \infty$. However, this limit vanishes exactly when f solves $t^2 - (f'(t)/f(t))^2 - 2[f'(t)/f(t)]' = E$, where E is a constant, that is the time-independent Schrödinger equation or quantum harmonic oscillator system, $-4\psi''(t) + t^2\psi(t) = E\psi(t)$ with $\psi(t) = \sqrt{f(t)}$, in our units. This happens exactly when f is a higher energy density. Therefore in this sense MIW sequences are approximately stable in the limit.

1.5. **Plan of the article.** After stating results and related remarks in Section 2, we give the proofs of Theorems 2.1, 2.3, 2.4, and 2.5 in Sections 3, 4, 5, and 6, referring at times to an appendix with technical lemmas.

1.6. **Notation.** We highlight some of the notation used in the article.

- $H_{MIW} = H$; time-independent Hamiltonian, (1.7).
- $(x_n)_{n=1}^N$; MIW sequence, with boundary conditions x_0, x_{N+1}, (1.10).
- f_ℓ; higher energy function of order ℓ, (1.12).

- p_ℓ; Hermite polynomial of order ℓ, (1.12).
- $R_k = (r_k, r_{k+1})$; intervals between zeroes $(r_k)_{k=0}^\ell$ of higher energy functions, with $r_0 = \infty$ and $r_{\ell+1} = \infty$, beginning of Sections 2, 3.3.
- N_k; number of MIW sequence points in R_k, Section 2.
- $d(\cdot, \cdot)$; Wasserstein-1 distance, Section 2.
- $n(t)$; maximal index of MIW sequence element x_n less than t, (2.1).
- χ_n; functions used to construct MIW sequences, beginning of Section 3.
- g_h; function used in Stein's equation, (5.1).
- $P = P_{a,b}$, $Q = Q_{a,b}$, and $R = R_{a,b}$; P is the distribution with density proportional to a higher energy function f_ℓ on an interval $R_k = (a, b)$, Q is the empirical distribution of the MIW sequence in (a, b), and R is an 'intermediate' distribution, beginning of Section 5.

2. RESULTS

Let f be a higher energy function of order $\ell \geq 0$, and when $\ell \geq 1$ let $r_1 < \cdots < r_\ell$ be its roots. Choose $N_k \geq 1$ for $0 \leq k \leq \ell$ when $\ell \geq 1$, and $N = N_0 \geq 2$ when $\ell = 0$. Denote the regions of strict positivity of f by R_0 for the region $(-\infty, r_1)$, by R_k for the region (r_k, r_{k+1}) when $1 \leq k < \ell$, and by R_ℓ for the region (r_ℓ, ∞).

In the following results, we will include the case $\ell = 0$ with respect to the Normal densities to be complete although, as discussed earlier, parts of Theorems 2.1, 2.3, 2.4 appear in [13], [5], [15]. We note the proof method for Theorem 2.4 for $\ell = 0$ differs from previous arguments.

We now state there is a unique MIW sequence matched to '$\mp\infty$' boundary conditions.

Theorem 2.1. *There is a unique MIW sequence $(x_n)_{n=1}^N$ of f that satisfies the left boundary condition at $x_0 = -\infty$, and the right boundary condition at $x_{N+1} = \infty$, with N_k points that lie in the region R_k for each $0 \leq k \leq \ell$, and $N = \sum_{k=0}^\ell N_k$.*

As a consequence, we deduce symmetry of MIW sequences when the number of points $N_k = N_{\ell-k}$ for $0 \leq k \leq \ell$. This condition automatically holds when $\ell = 0$, that is when f is the Normal density.

Corollary 2.2. *When $N_k = N_{\ell-k}$ for $0 \leq k \leq \ell$, the MIW sequence $(x_n)_{n=1}^N$ in Theorem 2.1 is symmetric in that $x_n = -x_{N-n+1}$ for $1 \leq n \leq N$.*

Proof. Let $y_n = -x_{N-n+1}$ for $1 \leq n \leq N$. By symmetry of the higher energy density f and that the number of points N_k in (r_k, r_{k+1}) is the same as the number in reflected region $(r_{\ell-k}, r_{\ell-k+1})$, $(y_n)_{n=1}^N$ is also an MIW sequence, satisfying left and right boundary conditions at $\mp\infty$, with the same number of points N as $(x_n)_{n=1}^N$. Therefore, by the uniqueness part of Theorem 2.1, $x_n = y_n$ for $1 \leq n \leq N$. $\square$

With respect to an MIW sequence, define now

$$n(t) = \max\left\{0 \leq k \leq N : x_k \leq t\right\} \tag{2.1}$$

as the closest member of $(x_n)_{n=1}^N$, with $x_0 = -\infty$ and $x_{N+1} = \infty$, to the left of $t \in \mathbb{R}$, or in other words $n(t)$ is the number of elements of $(x_n)_{n=1}^N$ less than or equal to t.

We state that 'gaps' $x_{n+1} - x_n$ vanish in the sequence, and give 'spanning' orders of x_1, x_N.

Theorem 2.3. *Consider the MIW sequence $(x_n)_{n=1}^N$ in Theorem 2.1 such that the numbers $N_k \uparrow \infty$ for $0 \leq k \leq \ell$. Then, for $t \in \mathbb{R}$, the difference $x_{n(t)+1} - x_{n(t)} \to 0$ as $N \uparrow \infty$. Consequentially, $\lim_{N\to\infty} x_{n(t)+1}^N = t$. Moreover, at the extremities, there is a constant $c > 0$ such that $c\sqrt{\log N} \leq |x_1|, x_N \leq c^{-1}\sqrt{\log N}$ for all large N.*

Given two probability distributions S, T on $\mathbb{R}$, the Wasserstein-1 distance can be defined $d(S, T) = \sup_h |\mathbb{E}_S[h] - \mathbb{E}_T[h]|$, where h ranges over the space of 1-Lipschitz functions. It can also be evaluated as $d(S, T) = \int_{\mathbb{R}} |F_S(x) - F_T(x)| dx$ where F_S, F_T are the respective distribution functions. By standard smoothing arguments, $d(S, T) = \sup_{h \in \mathcal{L}} |\mathbb{E}_S[h] - \mathbb{E}_T[h]|$, where $\mathcal{L}$ is the space of differentiable 1-Lipschitz functions h. We note that Wasserstein-1 distance convergence implies weak convergence.

We state convergence in the Wasserstein-1 distance of the empirical distribution of the sequence to the distribution with higher energy density f. Here, by convention, empty sums $\sum_{k=0}^{-1}$ vanish.

Theorem 2.4. *Let P denote the distribution on $\mathbb{R}$ with density f. Suppose the MIW sequence $(x_n)_{n=1}^N$ in Theorem 2.1 is such that $N_k = \lfloor N \int_{R_k} f(t)dt \rfloor$ for $0 \le k < \ell$ and $N_\ell = N - \sum_{k=0}^{\ell-1} N_k \ge \lfloor N \int_{R_\ell} f(t)dt \rfloor$. Then, the empirical distribution Q of $(x_n)_{n=1}^N$ converges to P with rate*

$$d(Q, P) = \sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_{P_N}[h]| = \mathcal{O}\left(\frac{\sqrt{\log N}}{N}\right).$$

as $N \uparrow \infty$.

Finally, we give a sense in which the sequence is an approximate critical point of H, and in this sense an approximate higher energy state.

Theorem 2.5. *The sequence $(x_n)_{n=1}^N$ in Theorem 2.1, such that the number of points $N_k \uparrow \infty$ for $0 \le k \le \ell$, is stationary in the limit, in the sense that, evaluated on $(x_n)_{n=1}^N$,*

$$\lim_{N \to \infty} \partial x_{n(t)} H = 0$$

for each $t \in \mathbb{R} \setminus \{r_1, \ldots, r_\ell\}$, away from any zeros of f.

2.1. Remarks. We have the following comments.

1. One might ask if one may construct MIW sequences for more general f, not necessarily a higher energy function. There may be applications for instance to numerical density approximation. Going through the proofs, one can see that the class of f's can be made wider, perhaps to 'log-concave' f's and to densities f supported on intervals, although this is not pursued here.

2. Also, we have taken $N_k \ge 1$ in Theorem 2.1, which means every interval (r_k, r_{k+1}) contains points of the MIW sequence. We believe with more work, and redefinition of the MIW sequence, one can take some of the intervals empty. But, given the application to approximation of the distributions with higher energy density f's, we have avoided this consideration.

3. In [5], a lower bound of $\mathcal{O}(\sqrt{\log N}/N)$ for the rate of Wasserstein-1 distance convergence of Q to P is shown in the Normal density, $\ell = 0$, setting. Convergence in Kolmogorov distance is also shown in [5]. It would be of interest to derive a lower bound to pair with the upper bound given in Theorem 2.4 when $\ell \ge 1$, as well to consider other distances.

4. Although the MIW sequences constructed are approximate higher energy states for H as stated in Theorem 2.5, they are not actual critical points of H, except when $\ell = 0$ (see the expression for $\partial_{x_n} H$ in Lemma 6.1). In fact, we observe in Lemma 6.3, with respect to $\ell = 1$, that $\partial_{x_n} H$ diverges at $x_n = x_{n(0)+1}$ as $N \uparrow \infty$ with rate $x_{n(0)+1}^{-3}$. In Lemma 6.2, we show that $x_{n(0)+1}$ is of order $N^{-1/3}$, from which we see $\partial_{x_{n(0)+1}} H$ diverges at order N. This is not a contradiction of Theorem 2.3, as $t = 0$ is a zero of the Maxwellian density.

In Figure 2, the $N = 5$ initial positions are given by the Maxwellian ($\ell = 1$) MIW sequence with three negative and two positive points. One can compare the time evolution of this sequence with that in Figure 1 which follows the dynamics starting from a different configuration with the same energy H. There is some indication that in a small time-scale that the MIW sequence is somewhat stationary (flatter trajectories). It would be of interest to understand better how well the evolved 'worlds' $(x_n(t))_{n=1}^N$ approximate the initial MIW sequence positions $(x_n = x_n(0))_{n=1}^N$.

5. Finally, in [11], MIW discrete Hamiltonian approximations of Schrödinger's equation with non-Harmonic potentials V are also discussed. From the proof discussion in Sections 1.4 and 6 we can infer more generally that convergence of the empirical distribution of MIW sequences to critical points should happen when $V(t) - (f'(t)/f(t))^2 - 2[f'(t)/f(t)]' = E$, the associated time-independent Schrödinger's equation. It would be of interest to investigate more carefully these convergences in this context.
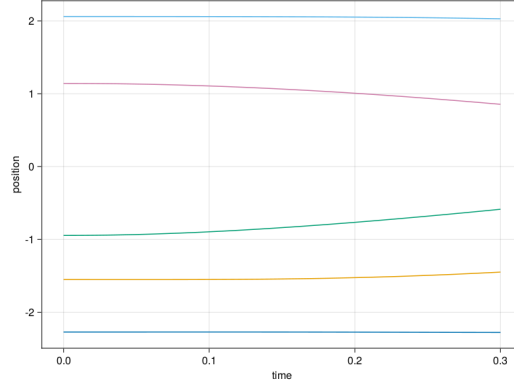
FIGURE 2. MIW $N = 5$ dynamics starting from the Maxwellian $\ell = 1$ approximating state $(x_n)_{n=1}^5$ with 3 negative and 2 positive values.

3. PROOF OF THEOREM 2.1: EXISTENCE AND UNIQUENESS OF MIW SEQUENCES

We will begin by defining an increasing sequence of functions $(\chi_n(x))_{n \geq 1}$, depending on a value $x \in \mathbb{R}$, whose evaluations satisfy the left boundary condition at $-\infty$, and the MIW recursion relation (1.10). Here, the parameter x will correspond to the first element of the sequence, $\chi_1(x) = x$. We will not consider the right boundary condition in defining this sequence, but will later choose x so that the sequence satisfies the right boundary condition at ∞.

These sequences, depending on the position of x, will lie entirely in a single region in which f is strictly positive. In order to create a sequence with points in *every* strictly positive region of f, we will use the single region existence to create a sequence in each region. The left boundary conditions will be chosen to allow the concatenation of these sequences to satisfy the MIW recursion relation.

We will then work from right to left. We choose the parameter of the last (say $\ell+1$th) sequence so that the $\ell + 1$th sequence satisfies the ∞-right boundary condition. Then, we choose the parameter of the ℓth sequence so that the concatenation of the ℓth and $\ell + 1$th sequences obeys the MIW recursion relation. We continue by choosing the parameter of the $(\ell - 1)$th sequence so that the concatenation of the $(\ell - 1)$th and ℓth sequences obeys the MIW recursion relation, and so on to the initial sequence, which a priori satisfies the $-\infty$-left boundary condition.

Uniqueness will be a consequence of the property that $\frac{d\chi_{n+1}}{d\chi_n} \geq 1$. This relation ensures that two sequences in the same strictly positive region of f with different initial values satisfy different right boundary conditions.

3.1. **Existence of the functions** χ_n. In the first step, we wish to define a family of functions $\chi_n(x)$ that correspond to an MIW sequence starting at $x \in (r, b_0)$, with a left boundary point of $a(x)$, leaving the right boundary undetermined. Here, r is a root of f or $r = -\infty$, and b_0 is the next root of f or $b_0 = \infty$ if there are no subsequent roots. It will be convenient to let $a(x) : (r, b_0) \to [-\infty, \infty)$ be a differentiable function such that $a(x) < x$ and $0 \leq \frac{da(x)}{dx} \leq 1$. We will also allow the choice of $a(x) \equiv -\infty$, with the convention in this case that $\frac{1}{x - a(x)} = 0$ for $x \in (r, b_0)$.

In the second step, we will match the final elements of these MIW sequences in (r, b_0) as left boundary points of MIW sequences in subsequent intervals. In this way, $a(x)$ for each sequence will be later identified.

For $x \in (r, b_0)$, define $\chi_1(x) = x$. We now construct functions $\chi_n(x)$ for $n \geq 1$ which will form the next elements of an MIW sequence. We want to choose b_1 so that (r, b_1) is the maximal domain of definition of $\chi_2(x)$.

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Lemma 3.1. *The minimum*

$$b_1 = \min\left\{x \in (r, b_0) \mid \frac{1}{x - a(x)} + \frac{f'(x)}{f(x)} = 0\right\}$$

is well-defined. Also, $\frac{1}{x-a(x)} + \frac{f'(x)}{f(x)} > 0$ *for* $x \in (r, b_1)$, $\lim_{x \downarrow r} \frac{1}{x-a(x)} + \frac{f'(x)}{f(x)} = \infty$, *and* $\lim_{x \uparrow b_1} \frac{1}{x-a(x)} + \frac{f'(x)}{f(x)} = 0$.

Proof. Because $0 \leq \frac{da(x)}{dx} \leq 1$ and $a(x) < x$, the quotient $\frac{1}{x-a(x)}$ is a decreasing, positive function of x. By Lemma A.3, the limit $\lim_{x \downarrow r} \frac{f'(x)}{f(x)} = \infty$. So, the limit of the sum $\lim_{x \downarrow r} \frac{1}{x-a(x)} + \frac{f'(x)}{f(x)} = \infty$.

Because b_0 is either a root of f or is infinite, again by Lemma A.3. the limit $\lim_{x \uparrow b_0} \frac{f'(x)}{f(x)} = -\infty$. Thus, the limit of the sum $\lim_{x \uparrow b_0} \frac{1}{x-a(x)} + \frac{f'(x)}{f(x)} = -\infty$.

Then, there is a point $b_1 \in (r, b_0)$ such that

$$\lim_{x \uparrow b_1} \frac{1}{x - a(x)} + \frac{f'(x)}{f(x)} = \frac{1}{b_1 - a(b_1)} + \frac{f'(b_1)}{f(b_1)} = 0.$$

Because $\frac{f'(x)}{f(x)}$ is strictly decreasing by Lemma A.2, we have that $\frac{1}{x-a(x)} + \frac{f'(x)}{/} f(x)$ is strictly decreasing for $x \in (r, b_0)$, the value b_1 is the unique such point.

Moreover, by this construction, $\frac{1}{x-a(x)} + \frac{f'(x)}{f(x)} > 0$ on (r, b_1). $\qquad\square$

We wish to mirror the recursion relation $x_2 = x_1 + \left(\frac{1}{x_1-a(x)} + \frac{f'(x_1)}{f(x_1)}\right)^{-1}$ of an MIW sequence. Thus, we define $\chi_2(x)$ on (r, b_1) as

$$\chi_2(x) = x + \left(\frac{1}{x - a(x)} + \frac{f'(x)}{f(x)}\right)^{-1}.$$

Base. In order to make an inductive definition for higher values of n, we will now note several properties of $\chi_1(x)$ and $\chi_2(x)$.

Lemma 3.2. *Define* b_0, b_1, χ_1, *and* χ_2 *as above. The following hold:*

(1) $r < b_1 < b_0$,
(2) $\chi_1(x)$ *is continuous for* $x \in (r, b_0)$,
(3) $\chi_2(x)$ *is continuous on* $x \in (r, b_1)$,
(4) $\chi_1(x) < \chi_2(x)$ *for all* $x \in (r, b_1)$,
(5) $\lim_{x \downarrow r} \chi_2(x) = r$, *and*
(6) $\lim_{x \uparrow b_1} \chi_2(x) = \infty$.

Proof. The first bullet holds because $b_1 \in (r, b_0)$. The second holds because $\chi_1(x) = x$. The third holds by inspection as b_1 was chosen to make (r, b_1) the maximal domain on which χ_2 is well-defined. The fourth holds because, after rearrangement, and noting Lemma 3.1,

$$\frac{1}{\chi_2(x) - \chi_1(x)} = \frac{f'(x)}{f(x)} + \frac{1}{\chi_1(x) - a(x)} > 0.$$

The fifth holds because $\lim_{x \downarrow r} \chi_1(x) = r$, and

$$\lim_{x \downarrow r} \frac{1}{\chi_2(x) - \chi_1(x)} = \lim_{x \downarrow r} \frac{f'(x)}{f(x)} + \frac{1}{\chi_1(x) - a(x)} = \infty$$

by Lemma 3.1. The sixth holds because $\lim_{x \uparrow b_1} \chi_1(x) = b_1$ is finite, and

$$\lim_{x \uparrow b_1} \frac{1}{\chi_2(x) - \chi_1(x)} = \lim_{x \uparrow b_1} \frac{f'(x)}{f(x)} + \frac{1}{\chi_1(x) - a(x)} = 0,$$

by Lemma 3.1 again. $\qquad\square$

Induction. Suppose we have successfully defined $\chi_{n-1}(x)$ and $\chi_n(x)$, on the domain (r, b_{n-1}), as we have done for $n = 2$. Suppose that for some $b_{n-2}, b_{n-1} \in \mathbb{R}$,

(1) $r < b_{n-1} < b_{n-2}$,
(2) $\chi_{n-1}(x)$ is continuous on $x \in (r, b_{n-2})$,
(3) $\chi_n(x)$ is continuous on $x \in (r, b_{n-1})$,
(4) $\chi_{n-1}(x) < \chi_n(x)$ for all $x \in (r, b_{n-1})$,
(5) $\lim_{x \downarrow r} \chi_n(x) = r$, and
(6) $\lim_{x \uparrow b_{n-1}} \chi_n(x) = \infty$.

We have already shown that these hold for the base case of $n = 2$.

We wish now to define b_n and the other items to complete induction. To begin with, we shall evaluate the limits of $\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))}$ at the boundary points of its domain to allow for an intermediate value argument.

Lemma 3.3. *The limit*

$$\lim_{x \downarrow r} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = \infty.$$

Proof. By assumption, $\chi_{n-1}(x) < \chi_n(x)$ in a neighborhood of r, and $\lim_{x \downarrow r} \chi_n(x) = \lim_{x \downarrow r} \chi_{n-1}(x) = r$. Then, $\lim_{x \downarrow r} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} = \infty$. Note also $\lim_{x \downarrow r} \frac{f'(\chi_n(x))}{f(\chi_n(x))} = \lim_{x \downarrow r} \frac{f'(x)}{f(x)} = \infty$, by Lemma A.3. The desired limit holds by adding the limits. $\qquad\square$

Note that the range of $\chi_n(x)$ is (r, ∞) for $x \in (r, b_{n-1})$. For $r < s < \infty$, let

$$\chi_n^{-1}(s) = \inf\{r < z < b_{n-1} : \chi_n(z) = s\}$$

be the generalized inverse. If $s = \infty$, let $\chi_n^{-1}(s) = b_{n-1}$. Note also, as b_0 is the next root of f after r, or $b_0 = \infty$ if no subsequent root exists, that $\chi_n^{-1}(b_0) \leq b_{n-1}$, and $f'(\chi_n(x))/f(\chi_n(x))$ is continuous for $x \in (r, \chi_n^{-1}(b_0))$.

Lemma 3.4. *The limit*

$$\lim_{x \uparrow \chi_n^{-1}(b_0)} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = -\infty.$$

Proof. The limit $\lim_{x \uparrow \chi_n^{-1}(b_0)} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} = \frac{1}{b_0 - \chi_{n-1}(\chi_n^{-1}(b_0))} < \infty$ as $\chi_n(x) > \chi_{n-1}(x)$ are continuous for $x \in (r, b_{n-1})$ by assumption. However, by Lemma A.3, we have that $\lim_{x \uparrow \chi_n^{-1}(b_0)} \frac{f'(\chi_n(x))}{f(\chi_n(x))} = -\infty$, yielding the result. $\qquad\square$

We now define b_n.

Lemma 3.5. *The value b_n is well-defined and given by*

$$r < b_n = \min\left\{ x \in (r, \chi_n^{-1}(b_0)) \mid \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = 0 \right\} < b_{n-1}.$$

Also, $\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} > 0$ *for* $x \in (r, b_n)$, *and* $\lim_{x \uparrow b_n} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = 0$.

Proof. By Lemma 3.3, the limit $\lim_{x \downarrow r} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = \infty$. As well, by Lemma 3.4, the limit $\lim_{x \uparrow \chi_n^{-1}(b_0)} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = -\infty$. Thus, by continuity of $\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + f'(\chi_n(x))/f(\chi_n(x))$ for $x \in (r, \chi_n^{-1}(b_0))$, following by assumption, there is a least intermediate point $r < b_n < \chi_n^{-1}(b_0) \leq b_{n-1}$, where

$$\lim_{x \uparrow b_n} \frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} = \frac{1}{\chi_n(b_n) - \chi_{n-1}(b_n)} + \frac{f'(\chi_n(b_n))}{f(\chi_n(b_n))} = 0.$$

Also, by construction, $\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} > 0$ for $x \in (r, b_n)$. $\qquad\square$

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We are now ready to define $\chi_{n+1}(x)$ for $x \in (r, b_n)$. Given $\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} > 0$ on (r, b_n) by Lemma 3.5, define

$$\chi_{n+1}(x) = \chi_n(x) + \left(\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} \right)^{-1}. \tag{3.1}$$

Lemma 3.6. *The function $\chi_{n+1}(x)$ is continuous and $\chi_{n+1}(x) > \chi_n(x)$ on (r, b_n).*

Proof. On the domain $(r, b_n) \subset (r, b_{n-1})$, the functions $\chi_{n-1}(x)$ and $\chi_n(x)$ are both continuous and $\chi_{n-1}(x) < \chi_n(x)$ by assumption. Hence, $\frac{1}{\chi_n(x) - \chi_{n-1}(x)}$ is continuous on (r, b_n). By the definition of b_n, $\frac{f'(\chi_n(x))}{f(\chi_n(x))}$ is continuous on (r, b_n). Moreover, by Lemma 3.5, $\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} > 0$ on (r, b_n). Thus, its reciprocal is continuous and positive on (r, b_n). Therefore, $\chi_{n+1}(x)$ is continuous and $\chi_{n+1}(x) > \chi_n(x)$ on (r, b_n). $\qquad\square$

We now wrap up the definition of χ_{n+1} by showing it satisfies the remaining properties required to complete the induction.

Lemma 3.7. *The limits $\lim_{x \downarrow r} \chi_{n+1}(x) = r$ and $\lim_{x \uparrow b_n} \chi_{n+1}(x) = \infty$.*

Proof. By assumption, $\lim_{x \downarrow r} \chi_n(x) = r$. Then, by Lemma 3.3, $\lim_{x \downarrow r} \frac{f'(\chi_n(x))}{f(\chi_n(x))} = \infty$. Since $\chi_n(x) > \chi_{n-1}(x)$ for $x \in (r, b_n) \subset (r, b_{n-1})$ by assumption, we have that $\lim_{x \downarrow r} \left(\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} \right)^{-1} = 0$. Hence, noting the definition of $\chi_{n+1}(x)$, the first limit holds.

Next, as $\chi_n(x)$ is continuous at $x = b_n \in (r, b_{n-1})$ by assumption, $\lim_{x \uparrow b_n} \chi_n(x) = \chi_n(b_n) < \infty$. Also, by Lemma 3.5, $\lim_{x \uparrow b_n} \left(\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} \right)^{-1} = \infty$. The second limit holds as a consequence. $\qquad\square$

For convenience, we summarize what we have shown via Lemmas 3.5, 3.6 and 3.7 in one place.

Proposition 3.8. *The following properties hold:*

(1) $r < b_n < b_{n-1}$,
(2) $\chi_n(x)$ *is continuous on* $x \in (r, b_{n-1})$,
(3) $\chi_{n+1}(x)$ *is continuous on* $x \in (r, b_n)$,
(4) $\chi_n(x) < \chi_{n+1}(x)$ *for all* $x \in (r, b_n)$,
(5) $\lim_{x \to r} \chi_{n+1}(x) = r$, *and*
(6) $\lim_{x \to b_n} \chi_{n+1}(x) = \infty$,

where recall that $r \in \mathbb{R}$ is a root of f, or $r = -\infty$, and b_0 is the next root after r of f, or if there no subsequent root, $b_0 = \infty$.

3.2. Properties of the functions χ_n.
In the following, let $N \geq 1$. Recall the definition of MIW sequence (1.10).

Lemma 3.9. *For $x \in (r, b_N)$, the sequence $(\chi_n(x))_{n=1}^N$ is an MIW sequence, satisfying the left boundary condition with boundary point $a(x)$, and the right boundary condition with boundary point $\chi_{N+1}(x)$. Moreover, for $x = b_N$, the sequence $(\chi_n(x))_{n=1}^N$ satisfies the right boundary condition with boundary ∞.*

Proof. By Lemma 3.6, the sequence is increasing, and the defining relation of $\chi_{n+1}(x)$ in (3.1) is the MIW recursion relation. Therefore, $(\chi_n(x))_{n=1}^N$ is an MIW sequence.

Rearranging the form of $\chi_2(x)$ in (3.1), we obtain $\frac{1}{\chi_2(x) - \chi_1(x)} - \frac{1}{\chi_1(x) - a(x)} = \frac{f'(\chi_1(x))}{f(\chi_1(x))}$, which is the left boundary condition at $a(x)$.

Also, by definition of $\chi_{N+1}(x)$ in (3.1), we have $\frac{1}{\chi_{N+1}(x) - \chi_N(x)} - \frac{1}{\chi_N(x) - \chi_{N-1}(x)} = \frac{f'(\chi_N(x))}{f(\chi_N(x))}$, which is the right boundary condition at $\chi_{N+1}(x)$.

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Finally, the point b_N is defined (Lemma 3.5) so that by continuity the relation

$$-\frac{1}{\chi_N(b_N) - \chi_{N-1}(b_N)} = \frac{f'(\chi_N(b_N))}{f(\chi_N(b_N))}$$

holds, which is the right boundary condition at ∞. □

The above development allows to construct an MIW sequence, with respect to higher energy functions, albeit in a single strictly positive region of f, on (r, b_0).

Lemma 3.10. *The sequence $(\chi_k(b_N))_{k=1}^N$ is an MIW sequence of f, bounded in the interval (r, b_0), satisfying the left boundary condition $a(x)$ and right boundary condition ∞. Moreover, For $n \geq 1$ and $x \in (r, b_n]$,*

$$r < \chi_1(x) < \cdots < \chi_n(x) < b_0.$$

We note $\chi_{n+1}(x)$ is defined for $x \in (r, b_n)$, however it is not bounded above, as $\lim_{x \uparrow b_n} \chi_{n+1}(x) = \infty$.

Proof. By Lemma 3.9, $(\chi_k(b_N))_{k=1}^N$ is an MIW sequence, satisfying the left and right boundary conditions.

Recall that $r < x = \chi_1(x) < \chi_k(x)$ for $2 \leq k \leq n$ on the interval $(r, b_n]$ (cf. Proposition 3.8). The lower bound in the second statement follows as a consequence.

For the upper bound, suppose $\chi_n(x_0) = b_0$ for some $x_0 \in (r, b_n]$. Note that $\chi_n(x_0) - \chi_{n-1}(x_0) > 0$, as $r < x_0 \leq b_n < b_{n-1}$, by Proposition 3.8 again. Also, $\lim_{x \uparrow b_0} f'(x)/f(x) = \infty$ by Lemma A.3. Then,

$$\chi_{n+1}(x_0) = \lim_{x \uparrow x_0} \chi_{n+1}(x) = \lim_{x \uparrow x_0} \chi_n(x) + \left(\frac{1}{\chi_n(x) - \chi_{n-1}(x)} + \frac{f'(\chi_n(x))}{f(\chi_n(x))} \right)^{-1} = \chi_n(x_0),$$

which contradicts the monotonicity $\chi_{n+1}(x) > \chi_n(x)$ for $r < x \leq b_n$ (cf. Proposition 3.8). Thus, $\chi_n(x) \neq b_0$. However, by Proposition 3.8, the limit $\lim_{x \downarrow r} \chi_n(x) = r < b_0$ and $\chi_n(x)$ is continuous for $x \in (r, b_n] \subset (r, b_{n-1})$. Therefore, $\chi_k(x) < \chi_n(x) < b_0$ for $1 \leq k \leq n-1$ and $x \in (r, b_n]$. □

When f is the Normal density, we have indeed constructed, as a direct consequence of Lemma 3.10, the desired MIW sequence, as also done in [13].

Corollary 3.11 (Normal $\ell = 0$). *Let $f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$. Choose $a(x) \equiv -\infty$. As f has no roots, $b_0 = \infty$. The sequence $(\chi_n(b_N))_{n=1}^N$, with $N \geq 2$, is an MIW sequence of f satisfying both the left boundary condition at $-\infty$, and right boundary condition at ∞.*

In Section 3.3, we will show how to construct sequences for higher energy f when $\ell \geq 1$. We now give two results that will be used to help define the choice of $a(x)$ in this respect.

Lemma 3.12. *For $1 \leq m \leq n$ and $x \in (r, b_{n-1})$, the derivative*

$$\frac{d\chi_n}{d\chi_m}(x) \geq 1.$$

In particular, as $\chi_1(x) = x$, we have $\frac{d\chi_n}{dx} \geq 1$ for $x \in (r, b_{n-1})$.

Proof. We will show first that $d\chi_{m+1}(x)/d\chi_m(x) \geq 1$. As a base case, when $m = 1$, the derivative

$$\frac{d\chi_2}{d\chi_1} = \frac{d}{d\chi_1} \left[\chi_1 + \left(\frac{1}{\chi_1 - a(x)} + \frac{f'(\chi_1)}{f(\chi_1)} \right)^{-1} \right]$$

$$= 1 - \left(\frac{1}{\chi_1 - a(x)} + \frac{f'(\chi_1)}{f(\chi_1)} \right)^{-2} \frac{d}{d\chi_1} \left(\frac{1}{\chi_1 - a(x)} + \frac{f'(\chi_1)}{f(\chi_1)} \right).$$

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The squared term is positive. It will be enough to show that $\frac{d}{d\chi_1}\left(\frac{1}{\chi_1 - a(x)} + \frac{f'(\chi_1)}{f(\chi_1)}\right)$ is negative. Because $\frac{da(x)}{dx} \leq 1$, and $\chi_1(x) = x$,

$$\frac{d}{d\chi_1}\frac{1}{\chi_1 - a(x)} = -(x - a(x))^{-2}\left(1 - \frac{da(x)}{dx}\right) \leq 0.$$

On the other hand, by log-concavity of f (Lemma A.2), the derivative $\frac{d}{d\chi_1}\frac{f'(\chi_1)}{f(\chi_1)} = \frac{d}{dx}\frac{f'(x)}{f(x)}$ is negative, finishing the base case.

For $m \geq 2$, the derivative

$$\frac{d\chi_{m+1}}{d\chi_m} = \frac{d}{d\chi_m}\left[\chi_m + \left(\frac{1}{\chi_m - \chi_{m-1}} + \frac{f'(\chi_m)}{f(\chi_m)}\right)^{-1}\right]$$

$$= 1 - \left(\frac{1}{\chi_m - \chi_{m-1}} + \frac{f'(\chi_m)}{f(\chi_m)}\right)^{-2}\frac{d}{d\chi_m}\left(\frac{1}{\chi_m - \chi_{m-1}} + \frac{f'(\chi_m)}{f(\chi_m)}\right).$$

Since $\left(\frac{1}{\chi_m - \chi_{m-1}} + \frac{f'(\chi_m)}{f(\chi_m)}\right)^{-2}$ is positive, once more we wish to show that $\frac{d}{d\chi_m}\left(\frac{1}{\chi_m - \chi_{m-1}} + \frac{f'(\chi_m)}{f(\chi_m)}\right)$ is negative. By the log-concavity of f again, the term $\frac{f'(\chi_m)}{f(\chi_m)}$ is decreasing as a function of χ_m, so its derivative with respect to χ_m is negative. But, the derivative

$$\frac{d}{d\chi_m}\frac{1}{\chi_m - \chi_{m-1}} = -(\chi_m - \chi_{m-1})^{-2}\frac{d}{d\chi_m}(\chi_m - \chi_{m-1})$$

$$= -(\chi_m - \chi_{m-1})^{-2}\left(1 - \frac{d\chi_{m-1}}{d\chi_m}\right) \leq 0,$$

since $\frac{d\chi_{m-1}}{d\chi_m} \leq 1$ by inductive assumption. Hence, $\frac{d\chi_{m+1}}{d\chi_m} \geq 1$.

Finally, to finish, we write

$$\frac{d\chi_n}{d\chi_m} = \prod_{k=m}^{n-1}\frac{d\chi_{k+1}}{d\chi_k} \geq 1. \qquad \square$$

Lemma 3.13. *For $n \geq 1$, the function $\chi_{n+1} : (r, b_n) \to (r, \infty)$ is invertible.*

Proof. The range of χ_{n+1} is well specified as $\lim_{x \to r}\chi_{n+1}(x) = r$, $\lim_{x \to b_n}\chi_{n+1}(x) = \infty$, and χ_{n+1} is continuous on (r, b_n) by Proposition 3.8. Since the derivative $\frac{d\chi_{n+1}}{dx} = \frac{d\chi_{n+1}}{d\chi_1} \geq 1$, we conclude that χ_{n+1} is strictly increasing and therefore invertible. $\qquad \square$

3.3. **Existence of MIW sequences for higher energy functions when $\ell \geq 1$.** Having found an MIW sequence with respect to the Normal density, $\ell = 0$, in Corollary 3.11, we fix $f(x)$ as a higher energy function of order $\ell \geq 1$ in this section. Let $r_0 = -\infty$, and $r_{\ell+1} = \infty$, where ℓ is the number of roots of $f(x)$. For $1 \leq k \leq \ell$, denote by r_k the kth root of $f(x)$. For each $0 \leq k \leq \ell$, choose a number $N_k \geq 1$ of points that lie in the region (r_k, r_{k+1}).

We will define sequences $(\chi_n(x))$ inductively on each strictly positive region of f. Here, x is a value in each region. We will denote by $(\chi_n^0(x))$ the sequence on the leftmost region, and by $(\chi_n^k(x))$ the sequence to the right of the kth root. Denote as well by $a_k(x)$ the choice of $a(x)$ for our kth sequence, that we will provide.

Base case. Define $\chi_n^0(x)$ by $\chi_n(x)$, as in Section 3.1 with $r = r_0$, $b_0 = r_1$ and $b_{n-1} = b_{n-1}^0$, on the subinterval (r_0, b_{n-1}^0) of (r_0, r_1). We want to satisfy the left boundary condition at $-\infty$, so we choose $a_0(x) \equiv -\infty$.

Induction. Suppose we have defined $\chi_n^k(x)$ on $(r_k, b_{N_k-1}^k) \subset (r_k, r_{k+1})$ for all $0 \leq k \leq K$. We wish for the left boundary condition of the next sequence to be the last element of the current one, that is, $a_{K+1}(y) = \chi_{N_K}^K(x)$, for some $x \in (r_K, r_{K+1})$, $y \in (r_{K+1}, r_{K+2})$ to be determined. As well, we

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wish for the first element of the next sequence to be the right boundary condition of the current one, $y = \chi_1^{K+1}(y) = \chi_{N_K+1}^K(x)$. In other words, informally,

$$(\chi_{N_K}^K)^{-1}(a_{K+1}(y)) = x \qquad \text{and} \qquad (\chi_{N_K+1}^K)^{-1}(y) = x,$$

or

$$(\chi_{N_K}^K)^{-1}(a_{K+1}(y)) = (\chi_{N_K+1}^K)^{-1}(y).$$

Thus, for $y \in (r_{K+1}, r_{K+2})$, we define

$$a_{K+1}(y) = \chi_{N_K}^K((\chi_{N_K+1}^K)^{-1}(y)).$$

Lemma 3.14. *The definition of a_{K+1} is well-defined. Moreover, $a_{K+1}(y) < y$ for $y \in (r_{K+1}, r_{K+2})$.*

Proof. Notice, by Lemma 3.13, for $y \in (r_{K+1}, r_{K+2}) \subset (r_K, \infty)$ that $x = (\chi_{N_K+1}^K)^{-1}(y) \in (r_K, b_{N_k}^K) \subset (r_K, b_{N_k-1}^K)$. Hence, x belongs to the domain of $\chi_{N_k}^K$, $a_{K+1}(y) = \chi_{N_k}^K(x) \in (r_K, \infty)$ is well-defined, and $(\chi_{N_k}^K)^{-1}(a_{K+1}(y)) = x$.

Moreover, as $x \in (r_K, b_{N_k}^K)$, by Lemma 3.10, we have $a_{K+1}(y) = \chi_{N_k}^K(x) < b_0^K = r_{K+1} < y$. $\square$

With this definition of a_{K+1}, it is ensured that if we take $x = (\chi_{N_K+1}^K)^{-1}(y)$, the concatenated sequence

$$\left(\chi_1^K(x), \ldots, \chi_{N_K}^K(x), \chi_1^{K+1}(y), \ldots, \chi_{N_K+1}^{K+1}(y) \right)$$

will be an MIW sequence.

We now complete the proof of the necessary properties of a_{K+1} to finish the induction step, namely $0 \le a_{K+1}'(y) \le 1$ for $y \in (r_{K+1}, r_{K+2})$, as we have already shown in Lemma 3.14 that $a_{K+1}(x) < x$ for $x \in (r_{K+1}, r_{K+2})$.

Lemma 3.15. *The bound $0 \le a_{K+1}'(x) \le 1$ holds for $x \in (r_{K+1}, r_{K+2})$.*

Proof. By Lemma 3.12, for $x \in (r_{K+1}, r_{K+2})$, $(\chi_{N_k+1}^K)^{-1}(x) \in (r_K, b_{N_k}^K)$ is differentiable. Also, for $y \in (r_K, b_{N_k}^K) \subset (r_K, b_{N_K-1}^K)$, $\chi_{N_K}^K(y)$ is differentiable. We compute the derivative

$$a_{K+1}'(x) = (\chi_{N_K}^K)'((\chi_{N_K+1}^K)^{-1}(x)) \; ((\chi_{N_K+1}^K)^{-1})'(x)$$

$$= \frac{(\chi_{N_K}^K)'((\chi_{N_K+1}^K)^{-1}(x))}{(\chi_{N_K+1}^K)'((\chi_{N_K+1}^K)^{-1}(x))} = \frac{(\chi_{N_K}^K)'(y)}{(\chi_{N_K+1}^K)'(y)},$$

where $y = (\chi_{N_K+1}^K)^{-1}(x)$. By Lemma 3.12, we have $\frac{d\chi_{N_K+1}^K}{d\chi_{N_K}^K} \ge 1$. Thus, $\frac{1}{a_{K+1}'(x)} = \frac{(\chi_{N_K+1}^K)'(y)}{(\chi_{N_K}^K)'(y)} \ge 1$ as well. Hence, both derivative bounds hold. $\square$

We now define $\chi_n^{K+1}(x)$ for $x \in (r_{K+1}, b_{n-1}^{K+1}) \subset (r_{K+1}, r_{K+2})$ as $\chi_n(x)$ with the choice $r = r_{K+1}$, $b_0 = r_{K+2}$, and $a_{K+1}(x) = \chi_{N_K}^K((\chi_{N_K+1}^K)^{-1}(x))$ to finish the induction step.

At this point, we have constructed an MIW sequence bridging the roots of f. What is left to choose is the value $x = x^K$ for each $\chi_n^K(x)$ for $1 \le K \le \ell$. These choices are limited by the concatenation relation. So, once a choice is made, say in the right-most interval, this choice is propagated backwards, determining the other choices all the way to the first interval.

As our first parameter, we choose $x^\ell = b_{N_\ell}^\ell$ to satisfy the right boundary condition at ∞, according to Lemma 3.9. Then, $x^{\ell-1} = (\chi_{N_{\ell-1}+1}^{\ell-1})^{-1}(x^\ell)$ is determined, so that the concatenation of the last two sequences will be an MIW sequence. Continuing recursively yields $x^{k-1} = (\chi_{N_{k-1}+1}^{k-1})^{-1}(x^k)$, for $1 \le k \le \ell$. The concatenation

$$(\chi_1^0(x^0), \ldots, \chi_{N_0}^0(x^0), \ldots, \chi_1^k(x^k), \ldots, \chi_{N_k}^k(x^k), \ldots, \chi_1^\ell(x^\ell), \ldots, \chi_{N_\ell}^\ell(x^\ell))$$

is then an MIW sequence of $f(x)$, with the desired number of points in each region, that satisfies both left and right boundary conditions at $\pm\infty$. We summarize this in the following proposition.

Proposition 3.16. *There is an MIW sequence of f that satisfies the left boundary condition at $-\infty$, and the right boundary condition at ∞, with $N_k \ge 1$ points that lie in the regions R_k for $0 \le k \le \ell$.*

3.4. **Uniqueness of MIW sequences for higher energy functions when $\ell \geq 0$.** Let now f be a higher energy function with order $\ell \geq 0$. When f has zeros, label them as $-\infty < r_1 < \cdots < r_\ell < \infty$. Denote by $r_0 = -\infty$ and $r_{\ell+1} = \infty$.

The MIW sequence $(x_n)_{n=1}^N$ constructed in Proposition 3.16 is in fact unique. Informally, we can see this from the uniqueness of the choices made during its construction. The choices of $a_k(x)$ are necessary to satisfy the recursion relation. The choice of x_ℓ is necessary to satisfy the right boundary condition. The choices of x_k for $0 \leq k < \ell$ are determined to satisfy the recursion relation.

We now proceed to show this more formally, using a different idea. We show that if the first elements of two sequences differ, then one of the two sequences does not satisfy the right boundary condition. Also, if the first elements are the same, then the two sequences are the same.

Note, when $\ell = 0$ and $N = 1$, as commented in the introduction, there is no one point MIW sequence (x_1) satisfying (1.10) with respect to left and right boundary conditions at $-\infty$ and ∞.

Lemma 3.17. *Consider two N-element MIW sequences, $(x_n)_{n=1}^N$ and $(y_n)_{n=1}^N$ satisfying the left $-\infty$ boundary condition, and x_{N+1}, y_{N+1} right boundary conditions respectively. Suppose for every $0 \leq k \leq \ell$, that both sequences have the same number of points $N_k \geq 1$ lying in the intervals (r_k, r_{k+1}) for $0 \leq k \leq \ell$.*

If $x_1 < y_1$, then $x_{n+1} - x_n < y_{n+1} - y_n$ for all $1 \leq n < N$. Consequentially $x_n < y_n$ for all $1 \leq n \leq N$.

On the other hand, if $x_1 = y_1$, then $x_n = y_n$ for $1 \leq n \leq N$.

Proof. When $N = 1$, the statement already holds.

Suppose $N \geq 2$. Because each sequence has the same number of points in each strictly positive region of f, the points x_n and y_n lie in the same region for every $1 \leq n \leq N$. As $x_1 < y_1$ lie in the same region and f is log-concave, we have $\frac{f'(y_1)}{f(y_1)} < \frac{f'(x_1)}{f(x_1)}$ (Lemma A.2). Then, with respect to the left boundary conditions,

$$\frac{1}{x_2 - x_1} = \frac{f'(x_1)}{f(x_1)} > \frac{f'(y_1)}{f(y_1)} = \frac{1}{y_2 - y_1}. \tag{3.2}$$

Thus, we can bound $x_2 - x_1 < y_2 - y_1$.

Suppose that $x_n < y_n$ and $x_{n+1} - x_n < y_{n+1} - y_n$ for some $1 \leq n < N$. This implies that $x_{n+1} < y_{n+1}$. Because x_{n+1} and y_{n+1} are in the same region, as before, $\frac{f'(y_{n+1})}{f(y_{n+1})} < \frac{f'(x_{n+1})}{f(x_{n+1})}$. Then,

$$\frac{1}{x_{n+2} - x_{n+1}} = \frac{1}{x_{n+1} - x_n} + \frac{f'(x_{n+1})}{f(x_{n+1})} > \frac{1}{y_{n+1} - y_n} + \frac{f'(y_{n+1})}{f(y_{n+1})} = \frac{1}{y_{n+2} - y_{n+1}}.$$

Thus, we can bound $x_{n+2} - x_{n+1} < y_{n+2} - y_{n+1}$. Hence, by this iteration, $x_n < y_n$ for $1 \leq n \leq N$.

The last statement follows the same argument: In (3.2), if $x_1 = y_1$, we would conclude $x_2 = y_2$, and so on. $\qquad \square$

Proposition 3.18. *There is at most one MIW sequence $(x_n)_{n=1}^N$ that satisfies the left boundary condition at $-\infty$ and the right boundary condition at ∞, with $N_k \geq 1$ points in the intervals (r_k, r_{k+1}) for $0 \leq k \leq \ell$ when $\ell \geq 1$, and $N = N_0 \geq 2$ when $\ell = 0$.*

Proof. Let $(x_n)_{n=1}^N$ and $(y_n)_{n=1}^N$ be two such sequences. If they are different, by Lemma 3.17, $x_1 \neq y_1$. To make a choice, suppose that $x_1 < y_1$. By Lemma 3.17, we have the relations $x_{n+1} - x_n < y_{n+1} - y_n$ for all $1 \leq n < N$, and thus $x_n < y_n$ for all $1 \leq n \leq N$. Our right boundary conditions require that

$$-\frac{1}{x_N - x_{N-1}} = \frac{f'}{f}(x_N) \qquad \text{and} \qquad -\frac{1}{y_N - y_{N-1}} = \frac{f'}{f}(y_N).$$

However, by log-concavity of f (Lemma A.2), $\frac{f'(x_N)}{f(x_N)} > \frac{f'(y_N)}{f(y_N)}$ and so $-\frac{1}{x_N - x_{N-1}} < -\frac{1}{y_N - y_{N-1}}$, or in other words $y_N - y_{N-1} < x_N - x_{N-1}$. This contradicts that $x_1 < y_1$. $\qquad \square$

Proof of Theorem 2.1. Existence follows from Corollary 3.11 for $\ell = 0$, and from Proposition 3.16 for $\ell \geq 1$. Uniqueness follows from Proposition 3.18. $\qquad \square$

4. Proof of Theorem 2.3: Gap sizes and span of MIW sequences

Suppose $f(x)$ is a higher energy function with order $\ell \geq 0$. When f has roots, label them as $r_1 < \cdots < r_\ell$. Let $r_0 = -\infty$ and $r_{\ell+1} = \infty$ By Theorem 2.1, let $(x_n)_{n=1}^N$ be the N-element MIW sequence of f satisfying the left boundary condition at $-\infty$, and the right boundary condition at ∞, such that in regions (r_k, r_{k+1}) there are $N_k \uparrow \infty$ points for $0 \leq k \leq \ell$. Note, when $\ell = 0$, the sequence $(x_n)_{n=1}^N$ is symmetric by Corollary 2.2 with $\lfloor N/2 \rfloor$ points below and above the origin.

Recall the definition of $n(t)$ in (2.1) as the index of the closest point in $(x_n)_{n=1}^N$ to the left of $t \in \mathbb{R}$. Recall also the MIW relation (1.10).

The strategy of proof of Theorem 2.3, at the end of the section, is to leverage the higher energy form of f, with $\ell + 1$ local maxima, which indicates that $x_2 - x_1$, $x_{n(r)+1} - x_{n(r)}$ for roots r, and $x_N - x_{N-1}$ are the local maxima of $x_{n+1} - x_n$ over $1 \leq n \leq N - 1$. Some development is needed to show these 'boundary' gaps vanish, as well as estimates for the orders of x_N, x_1 along the way in the following lemmas.

Lemma 4.1. *Let f be strictly positive on the finite interval (u, v) where u and v are consecutive zeros of f. Let $(x_n)_{n=1}^N$ be the part of an MIW sequence of f contained in (u, v). Then, $\lim_{N \to \infty} x_1 \to u$ and $\lim_{N \to \infty} x_N \to v$.*

Proof. Let $\varepsilon < 0$ be such that $\frac{1}{x_1 - u} \leq \frac{1}{\varepsilon}$, that is $x_1 \geq u + \varepsilon$. Note, as the left boundary point $x_0 \leq u$ that $\frac{1}{x_1 - x_0} \leq \frac{1}{\varepsilon}$. Moreover, by the form of f (cf. Lemma A.3), we can take ε smaller if necessary so that also $f'(u + \varepsilon) > 0$. Also, by log-concavity of f (Lemma A.2), $\frac{f'}{f}$ is decreasing on (u, v).

We can bound, as the MIW sequence $(x_n)_{n=1}^N$ is strictly increasing,

$$0 < \frac{1}{x_{n+1} - x_n} = \frac{1}{x_1 - x_0} + \sum_{k=1}^n \frac{f'(x_k)}{f(x_k)} \leq \frac{1}{\varepsilon} + n \frac{f'(u + \varepsilon)}{f(u + \varepsilon)}. \tag{4.1}$$

Then, by the MIW relation,

$$v - u \geq x_N - x_1 = \sum_{k=1}^{N-1} x_{k+1} - x_k \geq \sum_{k=1}^N \frac{1}{\frac{1}{\varepsilon} + k \frac{f'(u+\varepsilon)}{f(u+\varepsilon)}}.$$

The right hand side is diverges to ∞ as $N \to \infty$, yielding a contradiction. Hence, no such ε can exist. Therefore, for every $\varepsilon > 0$, for N sufficiently large, $u < x_1 < u + \varepsilon$.

The other limit holds by the same argument applied with the function $f(-x)$. $\qquad \square$

We now state an upperbound of x_N

Lemma 4.2. *Let f be strictly positive on (u, ∞) for $u = r_\ell$ when $\ell \geq 1$ and $u = 0$ when $\ell = 0$. Let $(x_n)_{n=1}^N$ denote the part of an MIW sequence of f contained in (u, ∞).*

Let $v > u$ be such that $p'_\ell(v)/p_\ell(v) \leq v/4$. Then, we have $x_N^2 \leq v^2 + 4(1 + \log N)$.

Proof. As $\frac{p'_\ell(x)}{p_\ell(x)} = O(1/x)$, we may find v be such that $\frac{1}{2}x \leq x - 2\frac{p'_\ell(x)}{p_\ell(x)}$ for $x \geq v$. Since $x_0 < u$, the index $n(v) \geq 0$.

If $N \leq n(v)$, the desired result holds trivially.

Suppose now $N - 1 \geq j \geq n(v)$,

$$0 < \frac{1}{2} \sum_{k=j+1}^N x_k \leq \sum_{k=j+1}^N x_k - 2\frac{p'_\ell(x_k)}{p_\ell(x_k)}.$$

Inverting both sides, noting the MIW sequence $(x_n)_{n=1}^N$ is increasing,

$$\frac{1}{\sum_{k=j+1}^N x_k - 2\frac{p'_\ell(x_k)}{p_\ell(x_k)}} \leq \frac{2}{\sum_{k=j+1}^N x_k} \leq \frac{2}{(N - j)x_{j+1}}. \tag{4.2}$$

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Note as $-f'(x)/f(x) = x - 2p'_\ell(x)/p_\ell(x)$, by the MIW relation (1.11), the fact $x_j < x_{j+1}$, and the last display (4.2) that

$$x_N^2 = x_{n(v)}^2 + \sum_{j=n(v)}^{N-1} x_{j+1}^2 - x_j^2 \leq x_{n(v)}^2 + 2 \sum_{j=n(v)}^{N-1} x_{j+1}(x_{j+1} - x_j)$$

$$= x_{n(v)}^2 + 2 \sum_{j=n(v)}^{N-1} \frac{x_{j+1}}{\sum_{k=j+1}^{N} x_k - 2\frac{p'_\ell(x_k)}{p_\ell(x_k)}} \leq x_{n(v)}^2 + 4 \sum_{j=n(v)}^{N-1} \frac{1}{N-j}.$$

Hence, $x_N^2 \leq x_{n(v)}^2 + 4(1 + \log(N - n(v))) \leq v^2 + 4(1 + \log N)$, as desired. $\qquad\square$

Lemma 4.3. *Let $\ell \geq 1$ and note f is strictly positive on (r_ℓ, ∞). Let $(x_n)_{n=1}^N$ be the part of an MIW sequence of f contained in (r_ℓ, ∞). Then, the limit $\lim_{N \to \infty} x_1 = r_\ell$ holds.*

Similarly, for $\ell \geq 1$, note f is strictly positive on $(-\infty, r_1)$. Let $(x_n)_{n=1}^N$ be the part of an MIW sequence contained in $(-\infty, r_1)$. Then, $\lim_{N \to \infty} x_N = r_1$.

Proof. Let $u = r_\ell$. Suppose $\varepsilon > 0$ is such that $\frac{1}{x_1 - u} \leq \frac{1}{\varepsilon}$, that is $x_1 \geq \varepsilon + u$. Hence, $x_j > x_1 \geq \varepsilon + u$ for $j \geq 1$. We can arrange by the form of f that also $f'(u + \varepsilon) > 0$ (cf. Lemma A.3). Following the proof of Lemma 4.1, noting (4.1), we have that

$$x_n \geq x_j + \sum_{k=j}^{n-1} \frac{1}{\frac{1}{\varepsilon} + k\frac{f'(u+\varepsilon)}{f(u+\varepsilon)}} \geq u + \sum_{k=j}^{n-1} \frac{1}{\frac{1}{\varepsilon} + k\frac{f'(u+\varepsilon)}{f(u+\varepsilon)}}. \tag{4.3}$$

Then, x_N must grow at least logarithmically with N. But, by Lemma 4.2 applied to the v specified there, we have $x_N^2 \leq v^2 + 4(1 + \log N)$, a contradiction of the lower order $\log N$ growth of x_N. Hence, $r_\ell = u < x_1 \leq u + \varepsilon$, and so $x_1 \to u$ as $N \uparrow \infty$.

The last statement follows the same argument by considering $f(u - x)$ for $u = r_1$. $\qquad\square$

We now give a lower bound for x_N.

Lemma 4.4. *Let f be strictly positive on (u, ∞) where $u = r_\ell$ if $\ell \geq 1$ and $u = 0$ when $\ell = 0$. Let $(x_n)_{n=1}^N$ denote the part of an MIW sequence of f contained in (u, ∞). Then, the term $x_N > \sqrt{\log N}$ as $N \uparrow \infty$.*

Proof. For $x > u$, we have $p'_\ell(x)/p_\ell(x) = \sum_{j=1}^{\ell}(x - r_j)^{-1} > 0$ when $\ell \geq 1$. When $\ell = 0$, $p'_\ell(x) = 0$. In both cases, $x - 2\frac{p'_\ell(x)}{p_\ell(x)} \leq x$.

Then, by (1.11) and as the MIW sequence $(x_n)_{n=1}^N$ is increasing,

$$0 < \frac{1}{x_{n+1} - x_n} = \sum_{k=n+1}^{N} x_k - 2\frac{p'_\ell(x_k)}{p_\ell(x_k)} \leq \sum_{k=n+1}^{N} x_k \leq (N - n)x_N.$$

That is to say, $\frac{1}{(N-n)x_N} \leq x_{n+1} - x_n$ for $1 \leq n \leq N - 1$.

Then, as $x_1 \geq 0$,

$$x_N = x_1 + \sum_{k=1}^{N-1} x_{k+1} - x_k \geq \sum_{k=1}^{N-1} \frac{1}{(N-k)x_N} = \frac{1}{x_N} \sum_{k=1}^{N-1} \frac{1}{k}.$$

Thus, we can bound $x_N^2 \geq \sum_{k=1}^{N-1} \frac{1}{k} \geq \log N$. $\qquad\square$

Lemma 4.5. *Let f be strictly positive in (u, ∞) where $u = r_\ell$ when $\ell \geq 1$ and $u = 0$ when $\ell = 0$. Let $(x_n)_{n=1}^N$ denote the part of an MIW sequence of f contained in (u, ∞). Then, for all N sufficiently large, $x_N - x_{N-1} < \frac{2}{\sqrt{\log N}}$.*

Similarly, with respect to the part of the MIW sequence contained in $(-\infty, v)$ where f is strictly positive and $v = r_1$ when $\ell \geq 1$ and $v = 0$ when $\ell = 0$, we have that $x_2 - x_1 < \frac{2}{\sqrt{\log N}}$.

Proof. Observe that $-\frac{f'(x)}{f(x)} = x - 2\frac{p'_\ell(x)}{p_\ell(x)} = x + \mathcal{O}(1/x)$ as $x \uparrow \infty$. Since $x_N \geq \sqrt{\log N}$ by Lemma 4.4, we have $x_N - 2\frac{p'_\ell(x_N)}{p_\ell(x_N)} \geq \frac{1}{2}x_N$ for large N. Thus, from the right ∞ boundary condition,

$$x_N - x_{N-1} = \frac{1}{x_N - 2\frac{p'_\ell(x_N)}{p_\ell(x_N)}} \leq \frac{2}{x_N} < \frac{2}{\sqrt{\log N}}.$$

The argument for $x_2 - x_1$ on the left end, follows by symmetry of f. $\qquad\square$

Lemma 4.6. *For each $t \in \mathbb{R}$, the difference $x_{n(t)+1} - x_{n(t)} \to 0$. Therefore, $\lim_{N\to\infty} x_{n(t)+1} = t$.*

Proof. Let m be a local maximum of f. Let r be the closest zero of f to the right of m, or if there is no such zero, let $r = \infty$. Similarly, let s be the closest zero to the left of m or if there is no such zero, let $s = -\infty$.

On the intervals (m, r) and (s, m), the function $\frac{f'(x)}{f(x)}$ is negative and positive respectively. Thus, given $x_k \in (m, r)$, by the MIW relation, $\frac{1}{x_{k+1}-x_k} - \frac{1}{x_k-x_{k-1}} = \frac{f'(x_k)}{f(x_k)} < 0$, or $x_k - x_{k-1} < x_{k+1} - x_k$. Likewise, given $x_k \in (s, m)$, we can bound $x_k - x_{k-1} > x_{k+1} - x_k$.

Hence, the interval sizes of $(x_n)_{n=1}^N$ are bounded by $x_{n(r)+1} - x_{n(r)}$ at roots r of f, or by $x_2 - x_1$ and $x_N - x_{N-1}$ at the extremities.

By Lemmas 4.1 and 4.3, $x_{n(r)+1} - x_{n(r)} \to 0$. By Lemma 4.5, applied with $u = r_\ell$, $v = r_1$ when $\ell \geq 1$ and with $u = v = 0$ when $\ell = 0$, $x_N - x_{N-1}, x_2 - x_1 \to 0$. Hence, for all $\ell \geq 0$, the gaps $x_{n(t)+1} - x_{n(t)} \to 0$ for $t \in \mathbb{R}$. $\qquad\square$

Proof of Theorem 2.3. The vanishing gap property is given in Lemma 4.6. The desired bound of x_N, and also of $|x_1|$ by symmetry of f, follow from Lemmas 4.2 and 4.4. $\qquad\square$

5. Proof of Theorem 2.4: Convergence in Wasserstein-1 distance

Let f be a higher energy function of order $\ell \geq 0$. Consider an interval (a, b) where f is strictly positive such that a is a zero of f or $a = -\infty$ and b is the next zero of f to the right of a or $b = \infty$. We will define $P = P_{a,b}$ as the distribution on (a, b) with density proportional to f. Consider the part of the MIW sequence constructed in Theorem 2.1 contained in (a, b), with $N = N_{a,b} \geq 2$ points, and denote it as $(x_n)_{n=1}^N$. Let $Q = Q_{a,b}$ be the empirical measure associated to this sequence.

Recall $n(t)$ defined in (2.1). To bound $|\mathrm{E}_P[h] - \mathrm{E}_Q[h]|$, as in [13, 5] with respect to the Normal density, we will compare Q with respect to another 'intermediate' continuous distribution $R = R_{a,b}$ with density

$$\rho(t) = \frac{1}{(N-1)(x_{n(t)+1} - x_{n(t)})},$$

supported on $(x_1, x_N) \subset (a, b)$.

Then, to compare R with P, we will use the 'differential equation' method with respect to a Stein equation. Define in terms of a differentiable 1-Lipschitz function $h \in \mathcal{L}$, the function

$$g_h(x) = \frac{1}{f(x)} \int_a^x f(t)(h(t) - \mathrm{E}_P[h]) \, dt. \tag{5.1}$$

Note that g_h satisfies the 'Stein equation',

$$g'_h(x) + \frac{f'(x)}{f(x)} g_h(x) = h(x) - \mathrm{E}_P[h]. \tag{5.2}$$

Such 'Stein equations' and subsequent approximations have been considered in wide generality; see [7], [8].

We will bound $|\mathrm{E}_R[h] - \mathrm{E}_Q[h]|$ in Section 5.1 and $|\mathrm{E}_R[h] - \mathrm{E}_P[h]|$ in terms of g_h in Section 5.2. Both will be shown, after development, of order $\mathcal{O}(\frac{x_N-x_1}{N})$.

On finite intervals $\frac{x_N-x_1}{N} = \mathcal{O}(1/N)$, and on infinite intervals, by Theorem 2.3, as $x_N, x_1 = \mathcal{O}(\sqrt{\log N})$, we have $\frac{x_N-x_1}{N} = \mathcal{O}(\sqrt{\log N}/N)$. We will piece together now these estimates over the

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intervals (r_k, r_{k+1}) between any zeros of f and conclude the proof of Theorem 2.4 in Section 5.9 that the Wasserstein-1 distance $d(P,Q) = \sup_{h \in \mathcal{L}} |E_P[h] - E_Q[h]| \leq \mathcal{O}(\frac{\sqrt{\log N}}{N})$, as desired.

It will be of later use to express the second derivative

$$g_h''(x) = -\left(\frac{f'(x)}{f(x)}\right)' g_h(x) - \left(\frac{f'(x)}{f(x)}\right) g_h'(x) + h'(x)$$

$$= 2\left(\frac{f'(x)}{f(x)}\right)^2 g_h(x) - \frac{f''(x)}{f(x)} g_h(x) - \frac{f'(x)}{f(x)}(h(x) - E_P[h]) + h'(x). \tag{5.3}$$

We also state a general estimate which will be helpful in the sequel, especially in places to bound terms uniformly over $h \in \mathcal{L}$.

Lemma 5.1. *Let P be a probability distribution on (a,b), where $-\infty \leq a < b \leq \infty$. Let h be a 1-Lipschitz function, and $y \in (a,b)$, Let also X be a random variable with distribution P.*
For $y \in \mathbb{R}$, we have $|h(y) - E_P[h]| \leq E_P|y - X| \leq |y| + E_P[|X|]$.
If a is finite, then $|h(y) - E_P[h]| \leq E_P[X] + y - 2a$.
If b is finite, then $|h(y) - E_P[h]| \leq 2b - E_P[X] - y$.
If a, b are both finite, then $|h(y) - E_P[h]| \leq b - a$

Proof. For $y \in (a,b)$, we compute, as $h \in \mathcal{L}$, that $|h(y) - E_P[h]| \leq E_P|y - X| \leq |y| + E_P[|X|]$. Moreover, if a is finite, then as $|y - X| \leq y - a + a - X$, we have $|h(y) - E_P[h]| \leq= E_P[X] + y - 2a$. Likewise, when b is finite, $|h(y) - E_P[h]| \leq 2b - E_P[X] - y$. Summing these, we obtain the last inequality, $2|h(y) - E_P[h]| \leq 2(b - a)$. $\square$

5.1. **Bound on $|E_R[h] - E_Q[h]|$.** Recall the distributions Q and R defined in terms of the MIW sequence $(x_n)_{n=1}^N$ of a higher energy function f. The following, in the case of the Normal density f, was started in [13, 5]. The argument is the same, given here for the reader's convenience.

Proposition 5.2. *We have that the Wasserstein-1 distance $\sup_{h \in \mathcal{L}} |E_R[h] - E_Q[h]| \leq \frac{x_N - x_1}{N-1}$.*

Proof. Let X be a random variable with distribution $Q = \frac{1}{N}\sum_{n=1}^N \delta_{x_n}$, and Y be a random variable with distribution R. We couple them as follows.

Choose a sequence $(z_n)_{n=1}^{N+1}$ such that $z_1 = x_1$, $z_{N+1} = x_N$, and $\int_{z_n}^{z_{n+1}} \rho(t)\, dt = \frac{1}{N}$. Since $\int_{x_k}^{x_{k+1}} \rho(t)\, dt = \frac{1}{N-1}$, we can bound $x_n \leq z_{n+1} \leq x_{n+1}$. Given $Y \sim R$, choose $X = x_{n^*(Y)}$, where $n^*(t) = \#\{z_k \leq t\}$. Then, $X \sim Q$, and $|Y - X| \leq x_{n^*(Y)+1} - x_{n^*(Y)}$.

Then, in terms of the coupled expectation $E_{Q,R}$,

$$\sup_{h \in \mathcal{L}} |E_R[h] - E_Q[h]| \leq E_{Q,R}|Y - X| \leq \sum_{n=1}^{N-1} \frac{x_{n+1} - x_n}{N-1} = \frac{x_N - x_1}{N-1}. \qquad \square$$

5.2. **Bound on $|E_R[h] - E_P[h]|$ in terms of g_h.** We show a bound between the intermediate distribution R and the continuous distribution $P = P_{a,b}$ restricted to an interval (a,b), in terms of g_h.

Proposition 5.3. *Let f be a higher energy function strictly positive on the interval (a,b), where a is a root of f or $a = -\infty$, and b is the next root after a or if there is no such root $b = \infty$. Let $(x_n)_{n=1}^N$ be part of an MIW sequence of f contained in (a,b).*
Then, for $\beta \in [0,1]$, and differentiable 1-Lipschitz $h \in \mathcal{L}$, we have

$$|E_R[h] - E_P[h]|$$

$$\leq \frac{1}{N-1}\left(\left|\frac{g_h(x_N)}{x_N - x_{N-1}} - \frac{g_h(x_1)}{x_2 - x_1} + \beta\left(\frac{f'}{f}g_h\right)(x_N) + (1-\beta)\left(\frac{f'}{f}g_h\right)(x_1)\right|\right.$$

$$\left. + (x_N - x_1)\left(1 + \sup_{x \in (x_1, x_N)} |g_h''(x)|\right)\right). \tag{5.4}$$

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Proof. Taking the expectation of each side of Stein's equation (5.2), with respect to R,

$$\mathrm{E}_R[h] - \mathrm{E}_P[h] = \int_a^b \rho(t)\left(g_h' + \frac{f'}{f}g_h\right)\,dt$$

$$= \sum_{n=1}^{N-1}\rho(x_n)\left(\int_{x_n}^{x_{n+1}}\frac{f'}{f}g_h\,dt + \int_{x_n}^{x_{n+1}}g_h'\,dt\right)$$

$$= \frac{1}{N-1}\left(\sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}}\frac{\left(\frac{f'}{f}g_h\right)(t)}{x_{n+1}-x_n}\,dt + \sum_{n=1}^{N-1}\frac{g_h(x_{n+1})-g_h(x_n)}{x_{n+1}-x_n}\right).$$

By summation by parts, as $\frac{1}{x_{n+1}-x_n} - \frac{1}{x_n-x_{n-1}} = \frac{f'(x_n)}{f(x_n)}$ by the MIW relation (1.10),

$$\sum_{n=1}^{N-1}\frac{g_h(x_{n+1})-g_h(x_n)}{x_{n+1}-x_n} = \frac{g_h(x_N)}{x_N-x_{N-1}} - \frac{g_h(x_1)}{x_2-x_1} - \sum_{n=2}^{N-1}\left(\frac{f'}{f}g_h\right)(x_n)$$

$$= \frac{g_h(x_N)}{x_N-x_{N-1}} - \frac{g_h(x_1)}{x_2-x_1} + \left(\frac{f'}{f}g_h\right)(x_1) - \sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}}\frac{\left(\frac{f'}{f}g_h\right)(x_n)}{x_{n+1}-x_n}\,dt. \qquad (5.5)$$

Instead of focusing on the left endpoint in (5.5), we can work with the right endpoint:

$$\left(\frac{f'}{f}g_h\right)(x_1) - \sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}}\frac{\left(\frac{f'}{f}g_h\right)(x_n)}{x_{n+1}-x_n}\,dt = \left(\frac{f'}{f}g_h\right)(x_N) - \sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}}\frac{\left(\frac{f'}{f}g_h\right)(x_{n+1})}{x_{n+1}-x_n}\,dt.$$

We may take a convex combination of the these expressions in terms of $\beta \in [0,1]$, and stick back into (5.5). Thus,

$$(N-1)|\mathrm{E}_R[h] - \mathrm{E}_P[h]|$$

$$\leq \left|\frac{g_h(x_N)}{x_N-x_{N-1}} - \frac{g_h(x_1)}{x_2-x_1} + \beta\left(\frac{f'}{f}g_h\right)(x_N) + (1-\beta)\left(\frac{f'}{f}g_h\right)(x_1)\right|$$

$$+ \beta\sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}}\frac{1}{|x_{n+1}-x_n|}\left|\left(\frac{f'}{f}g_h\right)(t) - \left(\frac{f'}{f}g_h\right)(x_{n+1})\right|\,dt$$

$$+ (1-\beta)\sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}}\frac{1}{|x_{n+1}-x_n|}\left|\left(\frac{f'}{f}g_h\right)(t) - \left(\frac{f'}{f}g_h\right)(x_n)\right|\,dt.$$

Define

$$K_h := \sup_{x,y\in(x_1,x_N)}\frac{1}{|y-x|}\left|\left(\frac{f'}{f}g_h\right)(y) - \left(\frac{f'}{f}g_h\right)(x)\right|.$$

We can compute, as $|x_{n+1}-x_n| = x_{n+1}-x_n$ as $(x_n)_{n=1}^N$ is increasing, that

$$\sum_{n=1}^{N-1}\sup_{s,t\in[x_n,x_{n+1}]}\left|\left(\frac{f'}{f}g_h\right)(t) - \left(\frac{f'}{f}g_h\right)(s)\right| \leq \sum_{n=1}^{N-1}K_h(x_{n+1}-x_n) = K_h(x_N-x_1).$$

Also, noting Stein's equation (5.2), and h is differentiable and 1-Lipschitz,

$$K_h \leq \sup_{x\in(x_1,x_N)}\left|\left(\frac{f'}{f}g_h\right)'\right| = \sup_{x\in(x_1,x_N)}|(h - \mathrm{E}_P[h] - g_h')'|$$

$$\leq \sup_{x\in(x_1,x_N)}|h'(x)| + |g_h''(x)| \leq 1 + \sup_{x\in(x_1,x_N)}|g_h''(x)|.$$

Putting these estimates together yields (5.4). $\qquad\square$

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5.3. Bounds of $\frac{f'(x_1)}{f(x_1)}g_h(x_1)$, $\frac{g_h(x_1)}{x_2-x_1}$ and $g_h''(x)$ near finite zeros of f. Let f be a higher energy function, strictly positive on (a,b), where $-\infty < a < b \leq \infty$. Suppose $f(a) = 0$, and h is a 1-Lipschitz differentiable function.

We begin with asymptotics near $x = a$, which will be helpful.

Lemma 5.4. *We have*

$$g_h(x) = \frac{1}{3}(x-a)(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)^2),$$

$$\frac{f'(x)}{f(x)}g_h(x) = \frac{2}{3}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)).$$

Here, $\mathcal{O}((x-a))$ and $\mathcal{O}((x-a)^2)$ do not depend on h.

Proof. Denote $F(x) = \int_a^x f(t)\,dt$. Integrating by parts,

$$\int_a^x f(t)(h(t) - \mathrm{E}_P[h])\,dt = F(x)(h(x) - \mathrm{E}_P[h]) - F(a)(h(a) - \mathrm{E}_P[h]) - \int_a^x F(t)h'(t)dt$$

$$= F(x)(h(x) - \mathrm{E}_P[h]) - \int_a^x F(t)h'(t)dt.$$

Using $f(x) = \frac{1}{2}f''(a)(x-a)^2 + \mathcal{O}((x-a)^3)$ for x near a (cf. Lemma A.1), which implies $F(x) = \frac{1}{6}f''(a)(x-a)^3 + \mathcal{O}((x-a)^4)$, $h'(x) = \mathcal{O}(1)$, and $h(x) - \mathrm{E}_P[h] = \mathcal{O}(x - 2a + \mathrm{E}_P[X]) = \mathcal{O}(1)$ (Lemma 5.1), we have

$$F(x)(h(x) - \mathrm{E}_P[h]) - \int_a^x F(t)h'(t)dt$$

$$= \frac{f''(0)}{6}(x-a)^3(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)^4) + \mathcal{O}((x-a)^4),$$

where $\mathcal{O}(\cdot)$ does not depend on h.

The first estimate now follows, noting again $h(x) - \mathrm{E}_P[X] = \mathcal{O}(1)$ for x near a, as

$$g_h(x) = \frac{\int_a^x f(t)(h(t) - \mathrm{E}_P[h])\,dt}{f(x)} = \frac{\frac{f''(a)}{6}(x-a)^3(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)^4)}{\frac{1}{2}f''(a)(x-a)^2 + \mathcal{O}((x-a)^3)}$$

$$= \frac{\frac{1}{3}(x-a)(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)^2)}{1 + \mathcal{O}((x-a))} = \frac{1}{3}(x-a)(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)^2),$$

where $\mathcal{O}(\cdot)$ does not depend on h.

The second estimate holds, noting the asymptotics of $f'(x)/f(x)$ near a in Lemma A.3, the first estimate of $g_h(x)$, and again $h(x) - \mathrm{E}_P[X] = \mathcal{O}(1)$:

$$\frac{f'(x)}{f(x)}g_h(x) = \left(\frac{2}{x-a} + \mathcal{O}(1)\right)\left(\frac{1}{3}(x-a)(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)^2)\right)$$

$$= \frac{2}{3}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x-a)),$$

where $\mathcal{O}(\cdot)$ does not depend on h. $\qquad\square$

With respect to a zero a of f, we know by Theorem 2.3 that the first MIW sequence element x_1 to the right of a satisfies $x_1 \to a$ as $N \uparrow \infty$.

Lemma 5.5. *Recall the setting of Proposition 5.3. Suppose a is finite. Then,*

$$\limsup_{N\uparrow\infty} \sup_{h\in\mathcal{L}} |\frac{f'(x_1)}{f(x_1)}g_h(x_1)| \leq \frac{2}{3}(\mathrm{E}_P[X] - a),$$

$$\limsup_{N\uparrow\infty} \sup_{h\in\mathcal{L}} \frac{|g_h(x_1)|}{x_2 - x_1} \leq \frac{5}{3}(\mathrm{E}_P[X] - a).$$

Proof. By Lemma 5.4 and Lemma 5.1, we bound $\limsup_{x \to a} \sup_{h \in \mathcal{L}} \left| \frac{f'(x)}{f(x)} g_h(x) \right| \leq \sup_{h \in \mathcal{L}} \frac{2}{3} |h(a) -$ $\mathrm{E}_P h| \leq \frac{2}{3}(\mathrm{E}_P[X] - a)$. The first limit now follows as a consequence as $x_1 \to a$ as $N \uparrow \infty$.

Next, recall the MIW boundary condition at $x_0 \leq a$: $\frac{1}{x_2-x_1} - \frac{1}{x_1-a} \leq \frac{1}{x_2-x_1} - \frac{1}{x_1-x_0} = \frac{f'(x_1)}{f(x_1)}$. Then,

$$\frac{|g_h(x_1)|}{x_2 - x_1} \leq \left(\frac{f'(x_1)}{f(x_1)} + \frac{1}{x_1 - a} \right) |g_h(x_1)| \leq \left| \frac{f'(x_1)}{f(x_1)} g_h(x_1) \right| + \frac{|g_h(x_1)|}{x_1 - a}.$$

By the definition of g_h and bound in Lemma 5.1, we have

$$\begin{aligned}
\frac{|g_h(x_1)|}{x_1 - a} &= \frac{1}{(x_1 - a)f(x_1)} \left| \int_a^{x_1} f(t)(h(t) - \mathrm{E}_P h) \, dt \right| \\
&\leq \frac{1}{(x_1 - a)f(x_1)} \int_a^{x_1} \sup_{s \in (a, x_1)} f(s) |h(s) - \mathrm{E}_P h| \, dt \\
&= \sup_{s \in (a, x_1)} \frac{f(s)}{f(x_1)} |h(s) - \mathrm{E}_P h| \leq \sup_{s \in (a, x_1)} \frac{f(s)}{f(x_1)} (s + \mathrm{E}_P[X] - 2a).
\end{aligned}$$

Observe as f has a root of order exactly 2 at a that $\sup_{s \in (a, x_1)} f(s)/f(x_1) \to 1$ as $N \uparrow \infty$. Consequently, uniformly over $h \in \mathcal{L}$, $\limsup_{N \uparrow \infty} \frac{|g_h(x_1)|}{x_1 - a} \leq \mathrm{E}_P[X] - a$.

Therefore, adding to the estimate from the first proven limit, we have

$$\lim_{x_1 \to a} \sup_{h \in \mathcal{L}} \frac{|g_h(x_1)|}{x_2 - x_1} \leq \frac{5}{3}(\mathrm{E}_P[X] - a). \qquad \square$$

We now bound $|g_h''(x)|$ near the zero a of f.

Lemma 5.6. *Recall the setting of Proposition 5.3. Suppose a is finite.*
Then, $\sup_{h \in \mathcal{L}} |g_h''(x)| = \mathcal{O}(1)$ for x near a.

Proof. Taking each part of the expression for g_h'' in the second line of (5.3) in turn, noting Lemmas A.3, 5.1, and 5.4,

$$\begin{aligned}
2 \left(\frac{f'(x)}{f(x)} \right)^2 g_h(x) &= 2 \left(\frac{2}{x - a} + \mathcal{O}(1) \right) \left(\frac{2}{3}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x - a)) \right) \\
&= \frac{8}{3}(x - a)^{-1}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}(1),
\end{aligned}$$

$$\begin{aligned}
-\frac{f''(x)}{f(x)} g_h(x) &= -\frac{f''(a) + \mathcal{O}((x - a))}{\frac{1}{2}f''(a)(x - a)^2 + \mathcal{O}((x - a)^3)} \left(\frac{1}{3}(x - a)(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x - a)^2) \right) \\
&= -(2(x - a)^{-2} + \mathcal{O}((x - a)^{-1})) \left(\frac{1}{3}(x - a)(h(x) - \mathrm{E}_P[h]) + \mathcal{O}((x - a)^2) \right) \\
&= -\frac{2}{3}(x - a)^{-1}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}(1),
\end{aligned}$$

and

$$\begin{aligned}
-\frac{f'(x)}{f(x)}(h(x) - \mathrm{E}_P[h]) &= -(2(x - a)^{-1} + \mathcal{O}(1))(h(x) - \mathrm{E}_P[h]) \\
&= -2(x - a)^{-1}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}(1).
\end{aligned}$$

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Then, the sum of these terms

$$g_h''(x) = \frac{8}{3}(x-a)^{-1}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}(1)$$

$$- \frac{2}{3}(x-a)^{-1}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}(1)$$

$$- 2(x-a)^{-1}(h(x) - \mathrm{E}_P[h]) + \mathcal{O}(1) + h'(x) = \mathcal{O}(1).$$

The terms $\mathcal{O}(\cdot)$ do not depend on h and $h'(x) = \mathcal{O}(1)$ for $h \in \mathcal{L}$. Hence, we can bound $|g_h''(x)| = \mathcal{O}(1)$, uniformly in $h \in \mathcal{L}$, for x near a. $\qquad\square$

Remark 5.7. We note that analogous results in Lemmas 5.5 and 5.6 hold on (a, b) where $-\infty \leq a < b < \infty$ with respect to finite right endpoints b which are zeros of f, by reordering the sequence right to left or say by considering $f(b - x)$. Recall the setting of Proposition 5.3. We have

$$\limsup_{N \uparrow \infty} \sup_{h \in \mathcal{L}} \left| \frac{f'(x_N)}{f(x_N)} g_h(x_N) \right| \leq \frac{2}{3}(b - \mathrm{E}_P[X]),$$

$$\limsup_{N \uparrow \infty} \sup_{h \in \mathcal{L}} \frac{|g_h(x_N)|}{x_N - x_{N-1}} \leq \frac{5}{3}(b - \mathrm{E}_P[X]),$$

$$\sup_{h \in \mathcal{L}} |g_h''(x)| = \mathcal{O}(1) \quad \text{for } x \sim b.$$

5.4. Bound of g_h'' at infinity. In this section, let f be a higher energy function strictly positive on (a, ∞), where a is a root of f or $a = -\infty$.

In the next two lemmas, we bound terms in the expression for g_h'' in the first line of (5.3).

Lemma 5.8. *We have*

$$\limsup_{x \to \infty} \sup_{h \in \mathcal{L}} \left| \left(\frac{f'(x)}{f(x)} \right)' g_h(x) \right| < \infty.$$

Proof. Recall that $P = P_{a,\infty}$ is the distribution with density proportional to f on (a, ∞). Since $\int_a^\infty (h(x) - \mathrm{E}_P[h]) f(x) dx = 0$, and $f(t)/f(x) = p_\ell^2(t) e^{-\frac{1}{2}t^2} / p_\ell^2(x) e^{-\frac{1}{2}x^2}$, we may write

$$p_\ell(x)^2 e^{-\frac{1}{2}x^2} g_h(x) = -\int_x^\infty (h(t) - \mathrm{E}_P[h]) p_\ell(t)^2 e^{-\frac{1}{2}t^2} \, dt. \qquad (5.6)$$

By Lemma 5.1, $|h(t) - \mathrm{E}_P[h]| \leq |t| + \mathrm{E}_P[|X|] \leq ct$ for large t. Since p_ℓ is an ℓ degree polynomial, we have also $c^{-1}t^\ell \leq p_\ell(t) \leq ct^\ell$ for large t. Moreover, by integration-by-parts, we have

$$\int_x^\infty t^{2\ell} t e^{-\frac{1}{2}t^2} dt = x^{2\ell} e^{-\frac{1}{2}x^2} \left(1 + \mathcal{O}(x^{-2})\right). \qquad (5.7)$$

Hence, $g_h(x) = \mathcal{O}(1)$ and, by Lemma A.3, $(f'(x)/f(x))'$ is of order $\mathcal{O}(1)$ for large x, where $\mathcal{O}(\cdot)$ does not depend on h. The result follows. $\qquad\square$

Lemma 5.9. *We have*

$$\limsup_{x \to \infty} \sup_{h \in \mathcal{L}} \left| \frac{f'(x)}{f(x)} g_h'(x) \right| < \infty.$$

Proof. Writing $g_h(x) = \frac{-1}{f(x)} \int_x^\infty f(t) (h(t) - \mathrm{E}_P[h]) dt$ (cf. (5.6)) and $g_h'(x) = h(x) - \mathrm{E}_P[h] - \frac{f'(x)}{f(x)} g_h(x)$ (cf. (5.2)), we have

$$\frac{f'(x)}{f(x)} g_h'(x) = \frac{f'(x)}{f(x)} (h(x) - \mathrm{E}_P[h]) + \left(\frac{f'(x)}{f(x)} \right)^2 \frac{1}{f(x)} \int_x^\infty f(t) (h(t) - \mathrm{E}_P[h]) dt. \qquad (5.8)$$

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Note, as $f(t) = p_\ell^2(t)e^{-\frac{1}{2}t^2}$,

$$\frac{1}{f(x)} \int_x^\infty f(t)\big(h(t) - \mathrm{E}_P[h]\big)dt = \frac{1}{f(x)} \int_x^\infty p_\ell^2(t)t^{-1}\big(h(t) - \mathrm{E}_P[h]\big)te^{-\frac{1}{2}t^2}dt$$

$$= \frac{1}{x}\big(h(x) - \mathrm{E}_P[h]\big) + \frac{1}{f(x)} \int_x^\infty \big(p_\ell^2(t)t^{-1}\big(h(t) - \mathrm{E}_P[h]\big)\big)'e^{-\frac{1}{2}t^2}dt.$$

Since $h'(t) = \mathcal{O}(1)$ and $|h(t) - \mathrm{E}_P[h]| = \mathcal{O}(t)$ by Lemma 5.1, we have

$$\big(p_\ell^2(t)t^{-1}\big(h(t) - \mathrm{E}_P[h]\big)\big)'$$
$$= 2p_\ell(t)p_\ell'(t)t^{-1}(h(t) - \mathrm{E}_P[h]) - p_\ell^2(t)t^{-2}(h(t) - \mathrm{E}_P[h]) + p_\ell^2(t)t^{-1}h'(t) = \mathcal{O}(t^{2\ell-1}).$$

By the scheme of (5.7), writing $t^{2\ell-1}e^{-t^2/2} = t^{2\ell-2}te^{-t^2/2}$, and as $f(x)$ is proportional to $x^{2\ell}e^{-x^2/2}\big(1 + \mathcal{O}(x^{-1})\big)$, we have

$$\frac{1}{f(x)} \int_x^\infty \big(p_\ell^2(t)t^{-1}\big(h(t) - \mathrm{E}_P[h]\big)\big)'e^{-\frac{1}{2}t^2}dt = \mathcal{O}(x^{-2}).$$

Now, $-f'(x)/f(x) = x + \mathcal{O}(x^{-1})$ by Lemma A.3. Inputting the above observations into (5.8), noting again that $x^{-1}\big(h(x) - \mathrm{E}_P[h]\big) = \mathcal{O}(1)$ by Lemma 5.1, we have

$$\frac{f'(x)}{f(x)}g_h'(x)$$
$$= \big(-x - \mathcal{O}(x^{-1})\big)\big(h(x) - \mathrm{E}_P[h]\big) + \big(x + \mathcal{O}(x^{-1})\big)^2\big(x^{-1}\big(h(x) - \mathrm{E}_P[h]\big) + \mathcal{O}(x^{-2})\big) = \mathcal{O}(1),$$

for all large x, uniformly in $h \in \mathcal{L}$. $\qquad\square$

Finally, we come to the bound of g_h''.

Lemma 5.10. *We have*

$$\limsup_{x\to\infty} \sup_{h\in\mathcal{L}} |g_h''(x)| < \infty.$$

Proof. By (5.3), we have $g_h''(x) = h'(x) - \left(\frac{f'(x)}{f(x)}\right)'g_h(x) - \left(\frac{f'(x)}{f(x)}\right)g_h'(x)$. For $h \in \mathcal{L}$, $|h'(x)| \leq 1$, and by Lemmas 5.8 and 5.9 the terms $\left(\frac{f'(x)}{f(x)}\right)'g_h(x)$ and $\left(\frac{f'(x)}{f(x)}\right)g_h'(x)$ are bounded $\mathcal{O}(1)$ for all large x, uniformly in h. Therefore, the claim follows. $\qquad\square$

5.5. Uniform bound of g_h'' in (x_1, x_N). Recall f is a higher energy function, strictly positive on (a, b) where a is a zero of f or $a = -\infty$, and b is the next zero of f or $b = \infty$. Let $(x_n)_{n=1}^N$ be part of an MIW sequence contained in (a, b).

Lemma 5.11. *We have*

$$\sup_{x\in(x_1,x_N)} \sup_{h\in\mathcal{L}} |g_h''(x)| < \infty.$$

Proof. Let $a < u < v < b$. Recall the formula for g_h'' in (5.3). We have $h'(x) = \mathcal{O}(1)$ and

$$g_h''(x) - h'(x) = 2\left(\frac{f'(x)}{f(x)}\right)^2 g_h(x) - \frac{f''(x)}{f(x)}g_h(x) - \frac{f'(x)}{f(x)}(h(x) - \mathrm{E}_P[h]).$$

As $|h(t) - \mathrm{E}_P[h]| \leq |t| + \mathrm{E}_P[|X|]$ by Lemma 5.1, we have

$$\sup_{x\in(u,v)} \sup_{h\in\mathcal{L}} |g_h(x)| \leq \sup_{x\in(u,v)} f^{-1}(x)\int_a^x (|t| + \mathrm{E}_P[|X|])f(t)dt < \infty.$$

Also, f'/f and f''/f are bounded on (u, v). Hence, $\sup_{x\in(u,v)} \sup_{h\in\mathcal{L}} |g_h''(x)| < \infty$.

Since g_h'' is bounded uniformly in h near a root by Lemma 5.6 and Remark 5.7, and at ∞ or $-\infty$ by symmetry of f via Lemma 5.10, the desired bound follows. $\qquad\square$

5.6. Wasserstein-1 distance bound on finite intervals.
We state a bound with respect to higher energy functions on a finite interval, bounded by zeroes.

Proposition 5.12. *Let f be a higher energy function, strictly positive on (a, b) where where $-\infty < a < b < \infty$ and a, b are zeros of f. Let P be the distribution for which f is the density, and Q be the empirical distribution of the part of the MIW sequence $(x_n)_{n=1}^N$ in (a, b).*

For all large N, the distance

$$d(Q, P) = \sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_P[h]| = \mathcal{O}\Big(\frac{1}{N}\Big).$$

Proof. Recall that $x_1 \to a$ and $x_N \to b$ as $N \to \infty$ by Theorem 2.3. Therefore, $x_N - x_1 \leq b - a$. Recall the intermediate continuous distribution R in Proposition 5.2, which bounds as a consequence $\sup_{h \in \mathcal{L}} |\mathrm{E}_R[h] - \mathrm{E}_Q[h]| = \mathcal{O}(1/N)$.

On the other hand, we bound $\sup_{h \in \mathcal{L}} |\mathrm{E}_R[h] - \mathrm{E}_P[h]|$ via the right-hand side of the estimate in Proposition 5.3. Here, it does not matter what the value $\beta \in [0, 1]$ is, but to be definite, we chose it as $\beta = 0$. By applying the bounds $|\frac{g_h(x_1)}{x_2 - x_1}| \leq 2(b - a)$, $|\frac{g_h(x_N)}{x_N - x_{N-1}}| \leq 2(b - a)$, and $|\frac{f'(x_1)}{f(x_1)} g_h(x_1)| \leq b - a$ in Lemma 5.5 and Remark 5.7, and the bound of $\sup_{x \in (x_1, x_N)} |g_h''(x)|$ in Lemma 5.11, we obtain $\sup_{h \in \mathcal{L}} |\mathrm{E}_R[h] - \mathrm{E}_P[h]| = \mathcal{O}(1/N)$.

Adding these two bounds, we obtain the desired estimate. $\qquad \square$

5.7. Wasserstein-1 distance bound on rays.
We now state a bound for higher energy functions on rays, where the finite endpoint is a zero.

Proposition 5.13. *Let f be a higher energy function, strictly positive on (a, ∞) (or $(-\infty, a)$) where a is a zero of f. Let P be the distribution for which f is the density, and Q be the empirical distribution of the part of the MIW sequence $(x_n)_{n=1}^N$ in (a, ∞) (or $(-\infty, a)$).*

For all large N, the distance

$$d(Q, P) = \sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_P[h]| = \mathcal{O}\Big(\frac{\sqrt{\log N}}{N}\Big).$$

Proof. We will concentrate on the case the ray is (a, ∞) as the same argument using $f(a - x)$ will apply to the ray $(-\infty, a)$. Recall that $x_1 \to a$ and $x_N = \mathcal{O}(\sqrt{\log N})$ as $N \to \infty$ by Theorem 2.3. Therefore, $x_N - x_1 = \mathcal{O}(\sqrt{\log N})$. Recall again the intermediate continuous distribution R in Proposition 5.2, which bounds $\sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_R[h]| = \mathcal{O}(\sqrt{\log N}/N)$.

We now take $\beta = 1$ in the inequality in Proposition 5.3 of $|\mathrm{E}_R[h] - \mathrm{E}_P[h]|$. Since the right boundary condition holds, $\frac{1}{x_N - x_{N-1}} = -\frac{f'(x_N)}{f(x_N)}$, we have that $\frac{g_h(x_N)}{x_N - x_{N-1}} + \big(\frac{f'}{f} g_h\big)(x_N) = 0$.

Hence, to bound the right-hand side in Proposition 5.3, we invoke Lemmas 5.5, 5.11 to bound $\frac{g_h(x_1)}{x_2 - x_1}$ and $\sup_{x \in (x_1, x_N)} |g_h''(x)|$. As a consequence, we obtain $\sup_{h \in \mathcal{L}} |\mathrm{E}_R[h] - \mathrm{E}_P[h]| = \mathcal{O}(\sqrt{\log N}/N)$.

Adding the bounds gives the result. $\qquad \square$

5.8. Wasserstein-1 distance bound for the Normal $\ell = 0$ case.
We rederive the bound found in [13, 5, 15], using the different 'density' approach.

Proposition 5.14 (Normal)**.** *Let f be the Normal density on $\mathbb{R}$, $f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2} x^2}$. Let P be the associated distribution. Let $(x_n)_{n=1}^N$ be the associated MIW sequence satisfying the left boundary condition at $-\infty$, and the right boundary condition at ∞, and Q its the empirical distribution.*

We have

$$d(Q, P) = \sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_{P_N}[h]| = \mathcal{O}\left(\frac{\sqrt{\log N}}{N}\right).$$

Proof. Note that $x_N, |x_1| = \mathcal{O}(\sqrt{\log N})$ by Theorem 2.3. Therefore, $x_N - x_1 = \mathcal{O}(\sqrt{\log N})$. Recall again the intermediate continuous distribution R in Proposition 5.2, which bounds $\sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_R[h]| = \mathcal{O}(\sqrt{\log N}/N)$.

Consider the bound in (5.4) with the choice $\beta = 1$. Again, because the right boundary condition at infinity is $\frac{g_h(x_N)}{x_N - x_{N-1}} = -\left(\frac{f'}{f} g_h\right)(x_N)$, we need only bound (1) $\sup_{h \in \mathcal{L}} \frac{|g_h(x_1)|}{x_2 - x_1} = \mathcal{O}(\sqrt{\log N})$, which requires a different argument than when the left endpoint of the interval is a zero of f, and (2) $\sup_{h \in \mathcal{L}} \sup_{x \in (x_1, x_N)} |g_h''(x)| = \mathcal{O}(1)$ which has already been shown in Lemma 5.11.

To this end, from the MIW relation, as $f'(x)/f(x) = -x$, we have $x_2 - x_1 = -x_1^{-1}$. Hence, we need to bound $|\frac{g_h(x_1)}{x_2 - x_1}| = |x_1 g_h(x_1)|$. Since $|h(t) - \mathrm{E}_P[h]| \le |t| + \mathrm{E}_P[|X|]$, we have

$$|x_1 g_h(x_1)| = \left| x_1 e^{\frac{1}{2}x_1^2} \int_{-\infty}^{x_1} e^{-\frac{1}{2}t^2} (h(t) - \mathrm{E}_P[h]) \, dt \right| \le 2|x_1| e^{\frac{1}{2}x_1^2} \int_{-\infty}^{x_1} e^{-\frac{1}{2}t^2} |t| \, dt,$$

for large N. As the term $x_1 \le 0$, we have

$$|x_1 g_h(x_1)| \le 2 x_1 e^{\frac{1}{2}x_1^2} \int_{-\infty}^{x_1} t e^{-\frac{1}{2}t^2} \, dt = -2x_1 = \mathcal{O}(\sqrt{\log N}). \qquad \square$$

5.9. **Wasserstein-1 distance bound for $\ell \ge 0$: Proof of Theorem 2.4.** We will break up f into strictly positive regions. We will then combine rates of convergence on each region, via the following lemma.

Proposition 5.15. *Let $P_{n,k}$ and P_k be probability distributions for $n \in \mathbb{N}$ and $0 \le k \le K$ for any $K \in \mathbb{N}$. Let $c_{n,k} > 0$ be such that $\sum_{k=0}^{K} c_{n,k} = 1$. Assume $\max_{0 \le k \le K} \int |x| \, dP_k < \mu < \infty$.*

Suppose, uniformly in k, $P_{n,k} \to P_k$ in the Wasserstein-1 metric with rate $r(n)$ and also c_k is such that $|c_{n,k} - c_k| \le r(n)$. Define mixture probability distributions $M_n = \sum_{k=0}^{K} c_{n,k} P_{n,k}$, and $M = \sum_{k=0}^{K} c_k P_k$.

Then, $d(M_n, M) \le (K + \mu) r(n)$.

Proof. Write, noting $|h(x) - h(0)| \le |x|$,

$$
\begin{aligned}
d(M_n, M) &= \sup_{h \in \mathcal{L}} \left| \int h \, dM_n - \int h \, dM \right| \\
&= \sup_{h \in \mathcal{L}} \left| \int (h - h(0)) \, dM_n - \int (h - h(0)) \, dM \right| \\
&\le \sum_{k=0}^{K} c_{n,k} \sup_{h} \left| \int (h - h(0)) \, dP_{n,k} - \int (h - h(0)) \, dP_k \right| + |c_{n,k} - c_k| \int |x| \, dP_k \\
&\le \sum_{k=0}^{K} c_{n,k} d(P_{n,k}, P_k) + r(n)\mu \ \le \ (K + \mu) r(n). \qquad \square
\end{aligned}
$$

Proof of Theorem 2.4. When $\ell = 0$, the result has been shown in Proposition 5.14.

Suppose now $\ell \ge 1$ when the function f has ℓ zeros, $r_1 < \cdots < r_\ell$. Let $r_0 = -\infty$ and $r_{\ell+1} = \infty$. Let $(x_n)_{n=1}^N$ be an N-element MIW sequence of f satisfying the left boundary condition at $-\infty$, and the right boundary condition at ∞. Suppose that in regions (r_k, r_{k+1}) there are $N_k = \lfloor N \int_{r_k}^{r_{k+1}} f_\ell(x) \, dx \rfloor$ many points for $0 \le k < \ell$ and $N_\ell = N - \sum_{k=0}^{\ell-1} N_k$ points in (r_ℓ, ∞). These sequences exist and are uniquely determined when $N_k \ge 1$ for $0 \le k \le \ell$ when $\ell \ge 1$ and $N = N_0 \ge 2$ when $\ell = 0$ by Theorem 2.1.

On each region (r_k, r_{k+1}), consider the subsequence contained, reordered, $(x_1, x_2, \cdots, x_{N_k})$. In the following, we will drop the subscript and call $N = N_k$. Denote as before by Q the empirical distribution of this subsequence and P the distribution with density proportional to f on (r_k, r_{k+1}). Recall the 'intermediate' continuous distribution R in Proposition 5.2.

On finite intervals (r_k, r_{k+1}), by Proposition 5.12 we have $d(Q, P) = \sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_P[h]| \le \frac{C}{N}$.

On the rays (r_ℓ, ∞) and $(-\infty, r_1)$, by Proposition 5.13, we have $d(Q, P) = \sup_{h \in \mathcal{L}} |\mathrm{E}_Q[h] - \mathrm{E}_P[h]| \le C \frac{\sqrt{\log N}}{N}$.

Note that the proportion of points in each region, $c_{N,k} = N_k/N$, differs from the probability $c_k = \int_{r_k}^{r_{k+1}} f dx$ of that region by $\mathcal{O}\left(\frac{1}{N}\right)$. Thus, we recover the statement in the theorem, by applying Proposition 5.15. $\qquad\square$

6. Proof of Theorem 2.5: Stability of the MIW sequences

We first give the proof of Theorem 2.5, and then make remarks on the behavior of the MIW sequence with respect to Maxwellian density, $\ell = 1$, at the zero $t = 0$, in Section 6.1.

Let $\eta(x) = \frac{f'(x)}{f(x)}$. The following notation will also be useful: Let $\nabla_n k = k_n - k_{n-1}$ with respect to a sequence $k = (k_n)_{n=1}^N$, and $\zeta_n = 1/\nabla_n x = 1/(x_n - x_{n-1})$ with respect to a sequence $x = (x_n)_{n=1}^N$. Then, $\eta(x_n) = \nabla_{n+1}\zeta = (x_{n+1} - x_n)^{-1} - (x_n - x_{n-1})^{-1}$ is a compact restatement of the MIW relation (1.10).

The gradient of H in (1.7) is computed as follows.

Lemma 6.1. *We have that*

$$\partial_{x_n} H = 2x_n - 2\frac{\eta(x_{n+1}) - \eta(x_n)}{(x_{n+1} - x_n)^2} + 2\frac{\eta(x_n) - \eta(x_{n-1})}{(x_n - x_{n-1})^2} \tag{6.1}$$

on an MIW sequence $(x_n)_{n=1}^N$ for f.

Proof. By the form of H, noting that only three terms in second sum of (1.7) depend on x_n,

$$\frac{1}{2}\partial_{x_n} H = x_n + (\nabla_n\zeta)\partial_{x_n}(\nabla_n\zeta) + (\nabla_{n+1}\zeta)\partial_{x_n}(\nabla_{n+1}\zeta) + (\nabla_{n+2}\zeta)\partial_{x_n}(\nabla_{n+2}\zeta)$$

$$= x_n + (\nabla_n\zeta)\partial_{x_n}\zeta_n + (\nabla_{n+1}\zeta)\partial_{x_n}\zeta_{n+1} - (\nabla_{n+1}\zeta)\partial_{x_n}\zeta_n - (\nabla_{n+2}\zeta)\partial_{x_n}\zeta_{n+1}$$

$$= x_n - \zeta_n^2\nabla_n\zeta + \zeta_{n+1}^2\nabla_{n+1}\zeta + \zeta_n^2\nabla_{n+1}\zeta - \zeta_{n+1}^2\nabla_{n+2}\zeta$$

$$= x_n - \zeta_{n+1}^2\left(\nabla_{n+2}\zeta - \nabla_{n+1}\zeta\right) + \zeta_n^2\left(\nabla_{n+1}\zeta - \nabla_n\zeta\right).$$

So far, we have not used the MIW relation $\nabla_{n+1}\zeta = \eta(x_n)$. Now, inputting this, we obtain directly (6.1). $\qquad\square$

Proof of Theorem 2.5. Taylor expansion of η, at a point x_n differing from a zero of f, gives

$$\frac{\eta(s) - \eta(x_n)}{(s - x_n)^2} = \frac{\eta'(x_n)}{s - x_n} + \frac{1}{2}\eta''(x_n) + r(s; x_n)$$

where the remainder $|r(s; x_n)| \leq |\eta'''(c)||s - x_n|$ with c between s and x_n.

Substituting into (6.1), with $s = x_{n+1}$ and also $s = x_{n-1}$, we obtain

$$\partial_{x_n} H = 2x_n - 2\eta'(x_n)\left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}}\right) - 2\eta''(x_n) - 2r(x_{n+1}; x_n) - 2r(x_{n-1}; x_n)$$

$$= 2x_n - 2\eta'(x_n)\eta(x_n) - 2\eta''(x_n) - 2r(x_{n+1}; x_n) - 2r(x_{n-1}; x_n). \tag{6.2}$$

Recall that $\lim_{N\to\infty} x_{n(t)} = t$, and the 'no gaps' property $\lim_{N\to\infty} x_{n+1} - x_n = 0$ holds by Theorem 2.3. Therefore $\lim_{N\to\infty} r(x_{n(t)+1}; x_{n(t)}) = 0$, for $t \in \mathbb{R}$ not equal to a zero of f. Plugging in $n(t)$ for n and taking the limit of both sides of (6.2) we have

$$\lim_{N\to\infty} \partial_{x_{n(t)}} H = 2t - 2\eta'(t)\eta(t) - 2\eta''(t).$$

Hence, for t away from zeros of f, $\lim_{N\to\infty} \partial_{n(t)} H = 0$ exactly when $(x^2 + \eta^2(x) - 2\eta'(x))' = 0$ or when there is a constant E such that

$$x^2 = 2\eta'(x) + \eta^2(x) + E. \tag{6.3}$$

However, the higher energy functions $f = cp_\ell^2(x)e^{-\frac{1}{2}x^2}$ satisfy (6.3) with $E = 4\ell + 2$, noting $p_\ell''(x) = xp_\ell'(x) - \ell p_\ell(x)$ and $\eta(x) = -x + \frac{2p_\ell'(x)}{p_\ell(x)}$, as

$$2\eta'(x) + \eta^2(x) + 4\ell + 2 = 4\frac{p_\ell''}{p_\ell} - 4x\frac{p_\ell'}{p_\ell} + x^2 + 4\ell = 4\frac{xp_\ell' - \ell p_\ell}{p_\ell} - 4x\frac{p_\ell'}{p_\ell} + x^2 + 4\ell = x^2.$$

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Therefore, we conclude the proof of Theorem 2.5. □

6.1. **Remarks on the form of stability.** We demonstrate, with respect to the Maxwellian density f, $\ell = 1$, that the convergence in Theorem 2.5 does not hold with $t = 0$, the zero of f. Note that $f'(x)/f(x) = -x + 2/x$. Consider the MIW sequence $(x_n)_{n=1}^N$ with equal numbers of points to the left and right of zero. By Corollary 2.2, such a sequence is symmetric. We will show in Lemma 6.3 that $\partial_{x_{n(0)+1}} H = -\partial_{x_{n(0)}} H$ diverges as $N \to \infty$.

First, although by Theorem 2.3, $x_{n(0)+1} \to 0$ as $N \uparrow \infty$, we give a rate in the following statement.

Lemma 6.2. *We have $x_{n(0)+1} = \mathcal{O}(1/N^{1/3})$ as $N \uparrow \infty$.*

An intuitive understanding of the rate $x_{n(0)+1} = \mathcal{O}(N^{-1/3})$ is as follows. By the MIW ansatz, $x_{n(0)+1}$ should approximate a $1/(N+1)$ quantile, that is one expects $\int_{x_{n(0)}}^{x_{n(0)+1}} f(t)\, dt = \mathcal{O}(1/N)$ as indeed follows, since $x_{n(0)+1} = -x_{n(0)}$, and $f(t) = \mathcal{O}(t^2)$ for $t \downarrow 0$.

Lemma 6.3. *The gradient of H, with respect to the Maxwellian density f, at $x_{n(0)+1}$ is of lower and upper order $x_{n(0)+1}^{-3}$, and therefore is bounded below of order N, by Lemma 6.2, as $N \uparrow \infty$.*

We first argue Lemma 6.3 and then Lemma 6.2.

Proof of Lemma 6.3. By explicit computation, applying the form of f in (6.1), we have

$$\frac{1}{2}\partial_{x_n} H = x_n + \frac{x_{n+1} - \frac{2}{x_{n+1}} - x_n + \frac{2}{x_n}}{(x_{n+1} - x_n)^2} - \frac{x_n - \frac{2}{x_n} - x_{n-1} + \frac{2}{x_{n-1}}}{(x_n - x_{n-1})^2}$$

$$= x_n + \frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}} - 2\frac{x_{n+1}^{-1} - x_n^{-1}}{(x_{n+1} - x_n)^2} + 2\frac{x_n^{-1} - x_{n-1}^{-1}}{(x_n - x_{n-1})^2}.$$

By the MIW relation, the right-hand side reduces to

$$\frac{2}{x_n} - 2\frac{x_{n+1}^{-1} - x_n^{-1}}{(x_{n+1} - x_n)^2} + 2\frac{x_n^{-1} - x_{n-1}^{-1}}{(x_n - x_{n-1})^2}. \tag{6.4}$$

After algebra,

$$-\frac{x_{n+1}^{-1} - x_n^{-1}}{(x_{n+1} - x_n)^2} = \frac{x_{n+1} - x_n}{x_n x_{n+1}(x_{n+1} - x_n)^2} = \frac{1}{x_n^2}\frac{x_n}{x_{n+1}(x_{n+1} - x_n)}$$

$$= \frac{1}{x_n^2}\frac{x_{n+1} - (x_{n+1} - x_n)}{x_{n+1}(x_{n+1} - x_n)} = \frac{1}{x_n^2}\left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_{n+1}}\right),$$

and likewise

$$\frac{x_n^{-1} - x_{n-1}^{-1}}{(x_n - x_{n-1})^2} = \frac{1}{x_n^2}\left(-\frac{1}{x_n - x_{n-1}} - \frac{1}{x_{n-1}}\right).$$

By these relations, and the MIW relation again, (6.4) becomes

$$\frac{2}{x_n} + \frac{2}{x_n^2}\left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_{n+1}} - \frac{1}{x_n - x_{n-1}} - \frac{1}{x_{n-1}}\right) = -\frac{2}{x_n^2}\left(\frac{1}{x_{n+1}} - \frac{2}{x_n} + \frac{1}{x_{n-1}}\right)$$

$$= \frac{2}{x_n^3}\left(1 - \frac{x_n}{x_{n+1}} - \left(\frac{x_n}{x_{n-1}} - 1\right)\right) = \frac{2}{x_n^3}\left(\frac{x_{n+1} - x_n}{x_{n+1}} - \frac{x_n - x_{n-1}}{x_{n-1}}\right).$$

Choose $n = n(0) + 1$. By symmetry, $x_{n(0)} = -x_{n(0)+1}$. So,

$$\frac{2}{x_{n(0)+1}^3}\left(\frac{x_{n(0)+2} - x_{n(0)+1}}{x_{n(0)+2}} - \frac{x_{n(0)+1} - x_{n(0)}}{x_{n(0)}}\right) = \frac{2}{x_{n(0)+1}^3}\left(\frac{x_{n(0)+2} - x_{n(0)+1}}{x_{n(0)+2}} + \frac{x_{n(0)+1} + x_{n(0)+1}}{x_{n(0)+1}}\right)$$

$$= \frac{2}{x_{n(0)+1}^3}\left(3 - \frac{x_{n(0)+1}}{x_{n(0)+2}}\right).$$

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Then, $\partial_{n(0)+1} H = \frac{4}{x_{n(0)+1}^3}\left(3 - \frac{x_{n(0)+1}}{x_{n(0)+2}}\right)$. Since $0 < x_{n(0)+1} < x_{n(0)+2}$, we conclude as desired

$$8x_{n(0)+1}^3 < \partial_{x_{n(0)+1}} H < 12x_{n(0)+1}^3. \qquad \square$$

Proof of Lemma 6.2. Multiply the MIW relation by x_n^2 and sum over n to obtain

$$\sum_{n=k+1}^{N} \frac{1}{x_n^2}\left(\frac{1}{x_{n+1} - x_n} - \frac{1}{x_n - x_{n-1}}\right) = \sum_{n=k+1}^{N} \frac{1}{x_n^2}\left(\frac{2}{x_n} - x_n\right).$$

Summing-by-parts on the left-hand side, and then rearranging, we obtain

$$\frac{1}{x_{k+1}^2}\frac{1}{x_{k+1} - x_k} = \sum_{n=k+1}^{N}\left(\frac{1}{x_n^2} - \frac{1}{x_{n+1}^2}\right)\frac{1}{x_{n+1} - x_n} - \sum_{n=k+1}^{N}\frac{1}{x_n^2}\left(\frac{2}{x_n} - x_n\right). \qquad (6.5)$$

Note

$$\left(\frac{1}{x_n^2} - \frac{1}{x_{n+1}^2}\right)\frac{1}{x_{n+1} - x_n} = \frac{x_n - x_{n+1}}{x_n^2 x_{n+1}^2} + \frac{2}{x_n^2 x_{n+1}},$$

and $\frac{-1}{x_n^2}\left(\frac{2}{x_n} - x_n\right) = \frac{1}{x_n} - \frac{2}{x_n^3}$. We also note by symmetry that $x_{n(0)+1} - x_{n(0)} = 2x_{n(0)+1}$.

Putting these things together, with $k = n(0)$, (6.5) multiplied by $2x_{k+1}^3$ becomes

$$1 = 2x_{k+1}^3 \sum_{n=k+1}^{N} \frac{1}{x_n} + 2x_{k+1}^3 \sum_{n=k+1}^{N} \frac{1}{x_n^2}\left(\frac{2}{x_{n+1}} - \frac{2}{x_n} + \frac{x_n - x_{n+1}}{x_{n+1}^2}\right).$$

Since the MIW sequence $(x_n)_{n=1}^{N}$ is increasing, and $x_n > 0$ for $n \geq k+1 = n(0)+1$, we have

$$x_{k+1}^3 \sum_{n=k+1}^{N} \frac{1}{x_{n+1}^2}\left|\frac{2}{x_{n+1}} - \frac{2}{x_n}\right| \leq x_{k+1}\sum_{n=k+1}^{N}\left(\frac{2}{x_n} - \frac{2}{x_{n+1}}\right) = \frac{2x_{k+1}}{x_{k+1}} = 2$$

and

$$x_{k+1}^3 \sum_{n=k+1}^{N} \frac{1}{x_{n+1}^2}\frac{|x_n - x_{n+1}|}{x_{n+1}^2} \leq x_{k+1}\sum_{n=k+1}^{N}\frac{x_{n+1} - x_n}{x_n x_{n+1}} = x_{k+1}\sum_{n=k+1}^{N}\left(\frac{1}{x_n} - \frac{1}{x_{n+1}}\right) = 1.$$

Therefore, we have

$$1 + 6 \geq 2Nx_{k+1}^3 \cdot \frac{1}{N}\sum_{n=k+1}^{N}\frac{1}{x_n}.$$

Moreover, we conclude $7 \geq 2Nx_{k+1}^3 \cdot \frac{1}{2}\int_0^\infty \frac{1}{t}\sqrt{\frac{8}{\pi}}t^2 e^{-\frac{1}{2}t^2}\,dt$ by Fatou's lemma, with respect to the weak convergence in Theorem 2.4, for all large N. The result now follows. $\qquad \square$

Appendix A. Properties of higher energy functions

We consider several properties of higher energy functions that will be needed.

Lemma A.1. *Suppose f is an nth order higher energy function. Then f has exactly n real roots. These roots are distinct, real, and have order two.*

Moreover, near a root a, $f(x) = \frac{1}{2}f''(a)(x-a)^2 + \mathcal{O}((x-a)^3)$ and $f'(x) = f''(a)(x-a) + \mathcal{O}((x-a)^2)$, where $f''(a) \neq 0$.

Proof. The Hermite polynomial $p_n(x) = e^{\frac{1}{2}x^2}g_n(x)$, where $g_n(x) = \frac{d^n}{dx^n}e^{-\frac{1}{2}x^2}$, has exactly n simple real roots, as g_n has exactly n simple real roots, which can be shown by induction. These are exactly the roots of $f(x) = cp_n^2(x)g_0(x)$ which are of order 2. The remaining statements follows by standard Taylor expansion. $\qquad \square$

Lemma A.2. *The higher energy functions are log-concave, in the sense that $(\log f)''(x) < 0$ when $(\log f)''(x)$ is defined.*

Proof. Let $f(x)$ be a higher energy function. The log-derivative $(\log f)'(x) = 2\frac{p_n'(x)}{p_n(x)} - x$. The term $-x$ is decreasing on $\mathbb{R}$. We will show that $\frac{p_n'(x)}{p_n(x)}$ is decreasing as well, for $x \in \mathbb{R}$ such that $p_n(x) \neq 0$. In the case $n = 0$, the normal case, p_n is constant, so it is decreasing.

Suppose the order of p_n is $n \geq 1$. We factor $p_n(x)$, $p_n(x) = \prod_{k=1}^{n}(x - r_i)$, where r_i are the roots of p_n. Then, $p_n'(x) = \sum_{j=1}^{n} \prod_{\substack{k=1 \\ j\neq k}}^{n}(x - r_i)$. Therefore, the quotient

$$\frac{p_n'(x)}{p_n(x)} = \frac{\sum_{j=1}^{n}\prod_{\substack{k=1 \\ j\neq k}}^{n}(x - r_i)}{\prod_{k=1}^{n}(x - r_i)} = \sum_{j=1}^{n}\frac{\prod_{\substack{k=1 \\ j\neq k}}^{n}(x - r_i)}{\prod_{k=1}^{n}(x - r_i)} = \sum_{j=1}^{n}\frac{1}{x - r_j}.$$

This is a sum of decreasing functions, and so $\frac{p_n'(x)}{p_n(x)}$ is decreasing. $\qquad\square$

Lemma A.3. *Let f be a higher energy function defined on $(-\infty, \infty)$. The limits $\lim_{x\to-\infty}\frac{f'(x)}{f(x)} = \infty$, and $\lim_{x\to\infty}\frac{f'(x)}{f(x)} = -\infty$. As well, if $f(r) = 0$ for some $r \in \mathbb{R}$, then $\frac{f'(x)}{f(x)} = \frac{2}{x-r} + O(1)$ as $x \to r$. In particular, $\lim_{x\to r^-}\frac{f'(x)}{f(x)} = -\infty$, and $\lim_{x\to r^+}\frac{f'(x)}{f(x)} = \infty$. Moreover, $f'(x)/f(x) = -x + \mathcal{O}(x^{-1})$ and $(f'(x)/f(x))' = 1 + \mathcal{O}(x^{-2})$ as $x \uparrow \infty$.*

Proof. As shown in the proof of Lemma A.2, we can write

$$\frac{f'(x)}{f(x)} = (\log f)'(x) = 2\frac{p_n'(x)}{p_n(x)} - x = 2\sum_{j=1}^{n}\frac{1}{x - r_j} - x.$$

As $x \to \pm\infty$, $f'(x)/f(x) \to \mp\infty$.

For a root r of f, the term $\frac{1}{x-r}$ is the only unbounded term near r. Hence, as $x \to r^-$, $f'(x)/f(x) \to -\infty$. Likewise, as $x \to r^+$, $f'(x)/f(x) \to \infty$.

Finally, the limits of $f'(x)/f(x)$ and $(f'(x)/f(x))'$ follow directly from the relation $f'(x)/f(x) = 2p_n'(x)/p(x) - x$. $\qquad\square$

Appendix B. Non-existence and non-uniqueness of MIW sequences

We discuss that it is not given that there is a unique MIW sequence matched to boundary conditions for say any smooth, strictly positive f.

Lemma B.1. *There is a smooth, strictly positive function f on $\mathbb{R}$ such that there is no MIW sequence of f with $N \geq 2$ points which satisfies the left boundary condition at $-\infty$.*

Proof. The left boundary condition at $-\infty$ is $\frac{1}{x_2 - x_1} = \frac{f'(x_1)}{f(x_1)}$, where $x_2 > x_1$. This has no solution if $\frac{f'(x_1)}{f(x_1)} = 0$, for instance if $f(x) \equiv 1$. $\qquad\square$

Lemma B.2. *There is a smooth, strictly positive integrable function f on $\mathbb{R}$ there are two distinct two-element MIW sequences of f which satisfy the left boundary condition at $-\infty$, and the right boundary condition at ∞.*

Proof. We will create an f such that both $(-2, -1)$ and $(1, 2)$ are MIW sequences of f satisfying the left boundary condition at $-\infty$, and the right boundary condition at ∞. Taking care of the positive side first, we require that $\frac{1}{2-1} = \frac{f'(1)}{f(1)}$ and that $-\frac{1}{2-1} = \frac{f'(2)}{f(2)}$. We can thus choose $f(x) = x$ in a neighborhood of one, and $f(x) = 3 - x$ is a neighborhood of two.

Likewise to satisfy the requirements at -2 and -1, we can choose $f(x) = -x$ in a neighborhood of -1, and $f(x) = 3 + x$ is a neighborhood of -2. Because f is specified only in the neighborhoods of finitely many points, and is smooth and strictly positive at those points, we can extend f to a smooth, strictly positive integrable function on $\mathbb{R}$. $\qquad\square$

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