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APPROXIMATE LINEAR RELATIONS FOR BESSEL FUNCTIONS*

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Abstract. In this study, we reveal an approximate linear relation for Bessel functions of the first kind, based on asymptotic analyses. A set of coefficients are calculated from a linear algebraic system. For any given error tolerance, a Bessel function of an order big enough is approximated by a linear combination of those with neighboring orders using these coefficients. This naturally leads to a class of ALmost EXact (ALEX) boundary conditions in atomic and multiscale simulations.

Keywords. Bessel function; asymptotic analysis; approximate linear relation; ALEX boundary condition.

AMS subject classifications. 33C10; 41A60.

1. Introduction

Bessel functions are a class of important special functions that arise in the study of mathematical physics [1–3]. For instance, the Laplace equation under cylindrical or spherical coordinates naturally leads to the Bessel functions as the component in the radial dimension.

In recent developments of atomic simulations for crystalline solids, Bessel functions serve as the kernel functions for one-way wave propagation. This evokes great interest in exploring the Bessel functions, which are key to the design of effective and accurate boundary conditions for atomic or multiscale simulations [4–7]. Furthermore, these functions also appear as the major part of kernel functions in a semi-discretized Schrödinger equation [8], and a semi-discretized Euler–Bernoulli beam equation [9]. For more discussions on boundary treatments of the Schrödinger equation, please refer to [10–12].

As is well-known, Bessel functions are linearly independent. No Bessel function of the first kind can be expressed as a linear combination of other Bessel functions of the first kind. However, we discover through asymptotic expansions that up to an arbitrarily small tolerance level, a Bessel function of the first kind with the order big enough, may be approximated by a linear combination of some other such functions. This yields accurate boundary conditions for the aforementioned applications, which are called ALmost EXact (ALEX) boundary conditions [8, 9].

In the rest of this paper, we shall first present the main theorem, and the proof using some lemmas in Section 2. Then in Sections 3 through 6, we shall prove the lemmas. In Section 7, we shall illustrate the high accuracy by numerical tests with the resulting ALEX boundary condition for a harmonic chain.

2. Main results

A Bessel function of the first kind $J_n(t)$ solves the following ordinary differential

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equation.

$$u'' + \frac{1}{t}u' + \left(1 - \frac{n^2}{t^2}\right)u = 0. \tag{2.1}$$

Its series expansion reads

$$J_n(t) = \sum_{k=0}^{+\infty} \frac{(-1)^k}{k!(n+k)!}\left(\frac{t}{2}\right)^{2k+n}. \tag{2.2}$$

The Bessel functions are linearly independent, namely, if a linear combination of any finitely many $J_n(t)$'s is zero, then all coefficients must be identically zero. This excludes the possibility of expressing a $J_n(t)$ by a linear combination of finitely many other Bessel functions of the first kind. However, if an arbitrarily small error tolerance is allowed, we may prove that such linear combinations exist.

Consider a set of numbers $\tilde{a}_k$ $(1 \le k \le L)$ with $L \ge 4$ satisfying the condition

$$\sum_{k=1}^{L} \tilde{a}_k k^l = \delta_{l,0}, \quad 0 \le l \le 3. \tag{2.3}$$

The main theorem for an approximate linear relation among Bessel functions is as follows.

THEOREM 2.1. *With $\tilde{a}_k$ $(1 \le k \le L)$ satisfying condition (2.3), for any given small $\varepsilon > 0$, there exists an integer N, such that for any $n > N$ and $t \in [0, +\infty)$, it holds that*

$$\left| \sum_{k=1}^{L} \tilde{a}_k J_{n-k}(t) - J_n(t) \right| < \frac{\varepsilon}{n^{\frac{1}{3}}}. \tag{2.4}$$

The proof is based on analysis over several intervals, which comprise the whole positive semi-axis for the temporal domain of the Bessel functions. To describe the decomposition of such intervals, we start with the following lemma.

LEMMA 2.1. *For any small $\varepsilon > 0$ and $n > \left[\frac{1}{\varepsilon^3}\right] + 1$, the equation*

$$e^{i\frac{\pi}{3}} \frac{J_{\frac{1}{3}}(-it)}{J_{-\frac{1}{3}}(-it)} = 6^{\frac{1}{3}} \frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{1}{3}\right)} \cdot \frac{n^{\frac{1}{3}} J_n(n) - \varepsilon}{n^{\frac{2}{3}} J_n'(n)} \tag{2.5}$$

has a real positive root $t_{n,\varepsilon}$ which is bounded from above by t_ε, the root to

$$e^{i\frac{\pi}{3}} \frac{J_{\frac{1}{3}}(-it)}{J_{-\frac{1}{3}}(-it)} = 1 - \frac{\sqrt{3}\pi}{6^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)}\varepsilon. \tag{2.6}$$

Here $[\cdot]$ denotes the integer part. The function on the left hand side of equation (2.5) is a real-valued function, and plotted in Figure 2.1. This lemma will be proved in Section 3.

We introduce $G^*(\varepsilon) = -\frac{1}{2}(3t_\varepsilon)^{\frac{2}{3}}$. For a small $\varepsilon > 0$ and given integer $n > \left[\frac{1}{\varepsilon^3}\right] + 1$, we refer to $[0, n - |G^*(\varepsilon)|n^{\frac{1}{3}}]$ as a precursory zone, $[n - |G^*(\varepsilon)|n^{\frac{1}{3}}, n + |G^*(\varepsilon)|n^{\frac{1}{3}}]$ as a major

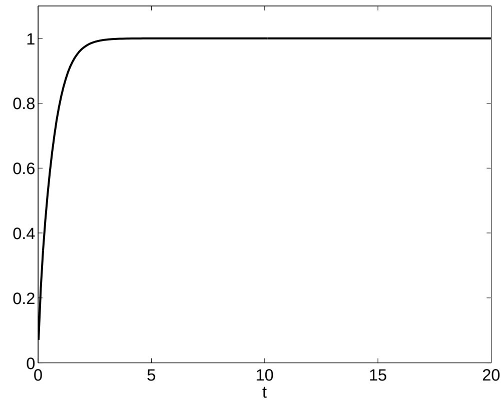

FIG. 2.1. *Function* $e^{i\frac{\pi}{3}}\frac{J_{\frac{1}{3}}(-it)}{J_{-\frac{1}{3}}(-it)}$.

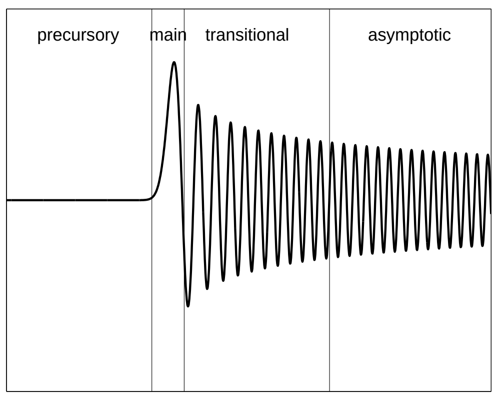

FIG. 2.2. *Schematic plot for a Bessel function and different zones.*

zone, $[n+|G^*(\varepsilon)|n^{\frac{1}{3}}, n+n^{\frac{1}{2}}]$ as a transitional zone, and $[n+n^{\frac{1}{2}}, +\infty)$ as an asymptotic zone. See Figure 2.2.

The asymptotic behaviors for the Bessel functions are stated as follows.

LEMMA 2.2. *For any* $\varepsilon > 0$, *there exists an integer* N *such that, for* $n \geq N$ *and* $t \in \left[0, n-|G^*(\varepsilon)|n^{\frac{1}{3}}\right]$, *it holds that* $0 \leq J_n(t) \leq \frac{\varepsilon}{n^{\frac{1}{3}}}$.

LEMMA 2.3. *Let a set of numbers* $\tilde{a}_k$ $(1 \leq k \leq L)$ *satisfy condition (2.3). There exists an integer* N *such that, for* $n \geq N$ *and* $t \in [n-|G^*(\varepsilon)|n^{\frac{1}{3}}, n+|G^*(\varepsilon)|n^{\frac{1}{3}}]$, *it holds that*

$$\left|\sum_{k=1}^{L} \tilde{a}_k J_{n-k}(t) - J_n(t)\right| \leq \frac{\varepsilon}{n^{\frac{1}{3}}}. \tag{2.7}$$

We remark that for $t \in [n-|G^*(\varepsilon)|n^{\frac{1}{3}}, n+|G^*(\varepsilon)|n^{\frac{1}{3}}]$, $J_n(t)$ is on the order of $O\left(\frac{1}{n^{\frac{1}{3}}}\right)$ [1]. With a coefficient ε, Lemma 2.3 presents an estimate of $\left|\sum_{k=1}^{L} \tilde{a}_k J_{n-k}(t) - J_{n-k}(t)\right|$, much better than that for $J_n(t)$.

LEMMA 2.4. *Let a set of numbers $\tilde{a}_k$ $(1\le k\le L)$ satisfy condition (2.3). For any $\varepsilon>0$, there exists an integer N such that, for $n\ge N$ and $t\in[n+|G^*(\varepsilon)|n^{\frac{1}{3}},n+n^{\frac{1}{2}}]$, it holds that*

$$\left|\sum_{k=1}^{L}\tilde{a}_k J_{n-k}(t)-J_n(t)\right|\le\frac{C(\varepsilon)}{n^{\frac{7}{6}}},\tag{2.8}$$

where $C(\varepsilon)$ depends on ε only.

On the interval $t\in[n+|G^*(\varepsilon)|n^{\frac{1}{3}},n+n^{\frac{1}{2}}]$, it is known that $J_n(t)=O\left(\frac{1}{n^\alpha}\right)$, with $\alpha\in\left[\frac{1}{3},\frac{3}{8}\right]$. Thus Lemma 2.4 presents an improved estimate for $\left|\sum_{k=1}^{L}\tilde{a}_k J_{n-k}(t)-J_n(t)\right|$.

LEMMA 2.5. *For any $\varepsilon>0$, there exists an integer N such that, for $n\ge N$ and $t\in[n+n^{\frac{1}{2}},\infty)$, it holds that*

$$J_{n-k}(t)=\sqrt{\frac{2}{\pi}}\cdot\frac{\cos\left(n\sqrt{\frac{t^2}{n^2}-1}-n\arctan\sqrt{\frac{t^2}{n^2}-1}+k\arctan\sqrt{\frac{t^2}{n^2}-1}-\frac{\pi}{4}\right)+R_{n,k}(t)}{\left(t^2-n^2\right)^{\frac{1}{4}}},\tag{2.9}$$

with $|R_{n,k}(t)|<\varepsilon$.

Now we prove Theorem 2.1.

Proof. For any small $\varepsilon>0$, from Lemma 2.2, we know there exists N_1 such that, for $n\ge N_1$ and $t\in\left[0,n-\left|G^*\left(\frac{\varepsilon}{1+A}\right)\right|n^{\frac{1}{3}}\right]$, it holds that

$$\left|\sum_{k=1}^{L}\tilde{a}_k J_{n-k}(t)-J_n(t)\right|\le\frac{\varepsilon}{(1+A)n^{\frac{1}{3}}}(1+A)<\frac{\varepsilon}{n^{\frac{1}{3}}}.\tag{2.10}$$

From Lemma 2.3, there exists N_2 such that, for $n\ge N_2$ and $t\in\Big[n-\left|G^*\left(\frac{\varepsilon}{1+A}\right)\right|n^{\frac{1}{3}},\ n+\left|G^*\left(\frac{\varepsilon}{1+A}\right)\right|n^{\frac{1}{3}}\Big]$, it holds that

$$\left|\sum_{k=1}^{L}\tilde{a}_k J_{n-k}(t)-J_n(t)\right|\le\frac{\varepsilon}{n^{\frac{1}{3}}}.\tag{2.11}$$

From Lemma 2.4, there exists $N_3>\left(\frac{C(\varepsilon)}{\varepsilon}\right)^{\frac{6}{5}}$ such that, for $n\ge N_3$ and $t\in\left[n+\left|G^*\left(\frac{\varepsilon}{1+A}\right)\right|n^{\frac{1}{3}},n+n^{\frac{1}{2}}\right]$, it holds that

$$\left|\sum_{k=1}^{L}\tilde{a}_k J_{n-k}(t)-J_n(t)\right|\le C(\varepsilon)n^{-\frac{7}{6}}\le\frac{\varepsilon}{n^{\frac{1}{3}}}.\tag{2.12}$$

From Lemma 2.5, there exists N_4 such that, for $n \geq N_4$ and $t \in \left[n+n^{\frac{1}{2}}, \infty\right)$, it holds that

$$\left|\sum_{k=1}^{L} \tilde{a}_k J_{n-k}(t) - J_n(t)\right| < O\left(\frac{1}{n^{\frac{3}{8}}}\right) \leq \frac{\varepsilon}{n^{\frac{1}{3}}}. \tag{2.13}$$

Now choose $N = \max(N_1, N_2, N_3, N_4)$, and let $n \geq N$. The inequality then holds over the whole domain $t \geq 0$. This completes the proof. □

In the above, we only require four linear constraints in condition (2.3). Making use of the freedom with $L > 4$, we may obtain better approximation by eliminating the leading term of the $J_n(t)$'s. For instance, we take $L = 30$ and introduce additional conditions as follows.

$$\sum_{k=1}^{30} \tilde{a}_k k^l \cos\frac{(k+l)\pi}{2} = \delta_{l,0}, \quad 0 \leq l \leq 3, \tag{2.14}$$

$$\sum_{k=1}^{30} \tilde{a}_k k^l \sin\frac{(k+l)\pi}{2} = 0, \quad 0 \leq l \leq 3, \tag{2.15}$$

$$\sum_{k=1}^{30} \tilde{a}_k \cos\frac{kl\pi}{20} = 1, \quad 1 \leq l \leq 9, \tag{2.16}$$

$$\sum_{k=1}^{30} \tilde{a}_k \sin\frac{kl\pi}{20} = 0, \quad 1 \leq l \leq 9. \tag{2.17}$$

Together with condition (2.3), we may fix the coefficients by solving the linear system.

In the following, we divide the asymptotic zone $[n+n^{\frac{1}{2}}, +\infty)$ into two subdomains, namely, $[n+n^{\frac{1}{2}}, n\sqrt{1+A_1}]$ and $[n\sqrt{1+A_1}, +\infty)$. Here we take

$$A = \sum_{k=1}^{L} |\tilde{a}_k|, \qquad A_1 = \left(\tan\left(\frac{1}{90A^{\frac{1}{9}}}\right)\right)^{-2}. \tag{2.18}$$

Lemma 2.6. *Let a set of numbers $\tilde{a}_k$ $(1 \leq k \leq 30)$ satisfy conditions (2.3), (2.14)-(2.17). For any $\varepsilon > 0$, there exists an integer N such that, for $n \geq N$ and $t \in [n+n^{\frac{1}{2}}, n\sqrt{1+A_1}]$, it holds that*

$$\left|\sum_{k=1}^{30} \tilde{a}_k J_{n-k}(t) - J_n(t)\right| < \sqrt{\frac{2}{\pi}} \frac{0.004+\varepsilon}{(t^2-n^2)^{\frac{1}{4}}}. \tag{2.19}$$

This gives an improved estimate for $\left|\sum_{k=1}^{30} \tilde{a}_k J_{n-k}(t) - J_{n-k}(t)\right|$.

Lemma 2.7. *For any $\varepsilon > 0$, there exists an integer N such that, for $n \geq N$ and $t \in \left[n\sqrt{1+A_1}, +\infty\right)$, it holds that*

$$J_{n-k}(t) = \sqrt{\frac{2}{\pi}} \left(\sqrt{t^2-n^2} - n\arctan\sqrt{\frac{t^2}{n^2}-1}\right)^{-\frac{1}{2}}.$$

$$\cos\left[\Phi - k\arctan\left(\frac{t^2}{n^2}-1\right)^{-\frac{1}{2}} + \frac{k\pi}{2}\right] + O\left(z^{-\frac{3}{2}}\right) \tag{2.20}$$

with a phase Φ given later, and

$$z = (n-k)\left(\sqrt{\frac{t^2}{(n-k)^2}-1} - \arctan\sqrt{\frac{t^2}{(n-k)^2}-1}\right). \tag{2.21}$$

Moreover, let a set of numbers $\tilde{a}_k$ $(1\le k\le 30)$ satisfy conditions (2.14)-(2.15). There exists N such that, for $n\ge N$ and $t\in\left[n\sqrt{1+A_1},+\infty\right)$, it holds that

$$\left|\sum_{k=1}^{30}\tilde{a}_k J_{n-k}(t) - J_n(t)\right| \le C\left(\sqrt{t^2-n^2} - n\arctan\sqrt{\frac{t^2}{n^2}-1}\right)^{-\frac{1}{2}}\left(\frac{t^2}{n^2}-1\right)^{-4} + O\left(z^{-\frac{3}{2}}\right), \tag{2.22}$$

where C is a constant.

This presents a better estimate of $\left|\sum_{k=1}^{30}\tilde{a}_k J_{n-k}(t) - J_{n-k}(t)\right|$ on $[n\sqrt{1+A_1},\infty)$.

We make some remarks. First, the conditions (2.16) and (2.17) come from the interpolation of $\sin kt$ and $\cos kt$ on $\left[0,\frac{\pi}{2}\right]$, which facilitate the asymptotic results in Lemma 2.6. Secondly, the conditions (2.14) and (2.15) are used in the analysis for Lemma 2.7. Please see the proofs for these two lemmas in Section 6. Finally, the number of terms matched in expressions (2.3)-(2.17) may be changed, and hence L may be chosen smaller accordingly.

In summary, for n large enough, we obtain estimates for $\left|\sum_{k=1}^{30}\tilde{a}_k J_{n-k}(t) - J_{n-k}(t)\right|$ smaller not only than $\frac{\varepsilon}{n^{\frac{1}{3}}}$ over the entire time axis, but also than $J_n(t)$'s leading term on each zone.

3. Precursory zone

In this section we prove Lemma 2.1 first.

Proof. The following asymptotic expansions hold for n large enough [3],

$$J_n(n) = \frac{1}{3\pi}\sin\frac{\pi}{3}\Gamma\left(\frac{1}{3}\right)\left(\frac{n}{6}\right)^{-\frac{1}{3}} + O\left(n^{-\frac{5}{3}}\right), \tag{3.1}$$

and

$$J_n'(n) = \frac{1}{3\pi}\sin\frac{2\pi}{3}\Gamma\left(\frac{2}{3}\right)\left(\frac{n}{6}\right)^{-\frac{2}{3}} + O\left(n^{-\frac{4}{3}}\right). \tag{3.2}$$

Straightforward calculations show that for given ε and large n the right-hand side of condition (2.3) becomes

$$1 - \varepsilon\frac{3\pi}{6^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\sin\frac{\pi}{3}} + O\left(n^{-\frac{2}{3}}\right). \tag{3.3}$$

Noticing $n > \left[\frac{1}{\varepsilon^3}\right]+1$, we have $O\left(n^{-\frac{2}{3}}\right)$ is contained within $O(\varepsilon^2)$.

For $t>0$, both $e^{-i\frac{\pi}{6}}J_{\frac{1}{3}}(-it)$ and $e^{i\frac{\pi}{6}}J_{-\frac{1}{3}}(-it)$ are pure imaginary [1]. From

$$e^{-i\frac{\pi}{6}}J_{\frac{1}{3}}(-it)\sim\frac{e^t}{\sqrt{2\pi}\Gamma\left(\frac{5}{6}\right)}\sum_{k=0}^{+\infty}\frac{\Gamma\left(k+\frac{5}{6}\right)}{12^k k!t^{k+\frac{1}{2}}},\tag{3.4}$$

$$e^{i\frac{\pi}{6}}J_{-\frac{1}{3}}(-it)\sim\frac{e^t}{\sqrt{2\pi}\Gamma\left(\frac{1}{6}\right)}\sum_{k=0}^{+\infty}\frac{5^k\Gamma\left(k+\frac{1}{6}\right)}{12^k k!t^{k+\frac{1}{2}}},\tag{3.5}$$

the left-hand side of equation (2.5) becomes

$$e^{i\frac{\pi}{3}}\frac{J_{\frac{1}{3}}(-it)}{J_{-\frac{1}{3}}(-it)}=\frac{1+\frac{5}{72t}+O\left(\frac{1}{t^2}\right)}{1+\frac{5}{72t}+O\left(\frac{1}{t^2}\right)}.\tag{3.6}$$

Therefore the left-hand side of equation (2.5) tends to 1 as $t\to+\infty$, and equals to 0 when $\theta=0$. Because of continuity, equation (2.6) has at least one root denoted as t_ε, which depends on ε but not n. Equation (2.5) has the same left-hand side as equation (2.6), and a smaller right hand side

$$1-\varepsilon\frac{3\pi}{6^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\sin\frac{\pi}{3}}+O\left(\varepsilon^2\right)\le 1-\varepsilon\frac{3\pi}{2\cdot 6^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)\sin\frac{\pi}{3}}=1-\frac{\sqrt{3}\pi}{6^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)}\varepsilon,\tag{3.7}$$

for small ε. Therefore, again because of continuity, equation (2.5) has at least one root $t_{n,\varepsilon}$ smaller than t_ε. ∎

Next, we prove Lemma 2.2.

Proof. From Equation (2.1), by direct calculations we find that for a given $\varepsilon>0$, the functions

$$u_1(\theta)=J_n(ne^\theta)-\frac{\varepsilon}{n^{\frac{1}{3}}},\tag{3.8}$$

$$\begin{aligned}u_2(\theta)=(2\theta)^{\frac{1}{2}}\Bigg[&\Gamma\left(\frac{2}{3}\right)\left(\frac{n}{6}\right)^{\frac{1}{3}}\left(J_n(n)-\frac{\varepsilon}{n^{\frac{1}{3}}}\right)J_{-\frac{1}{3}}\left(\frac{n(2\theta)^{\frac{3}{2}}}{3}\right)\\&+\Gamma\left(\frac{1}{3}\right)\left(\frac{n}{6}\right)^{\frac{2}{3}}J_n'(n)J_{\frac{1}{3}}\left(\frac{n(2\theta)^{\frac{3}{2}}}{3}\right)\Bigg],\end{aligned}\tag{3.9}$$

solve respectively the equations

$$\frac{d^2}{d\theta^2}u_1(\theta)+n^2(e^{2\theta}-1)u_1(\theta)+\frac{\varepsilon}{n^{\frac{1}{3}}}n^2(e^{2\theta}-1)=0,\tag{3.10}$$

$$\frac{d^2}{d\theta^2}u_2(\theta)+2n^2\theta u_2(\theta)+2\frac{\varepsilon}{n^{\frac{1}{3}}}n^2\theta=0.\tag{3.11}$$

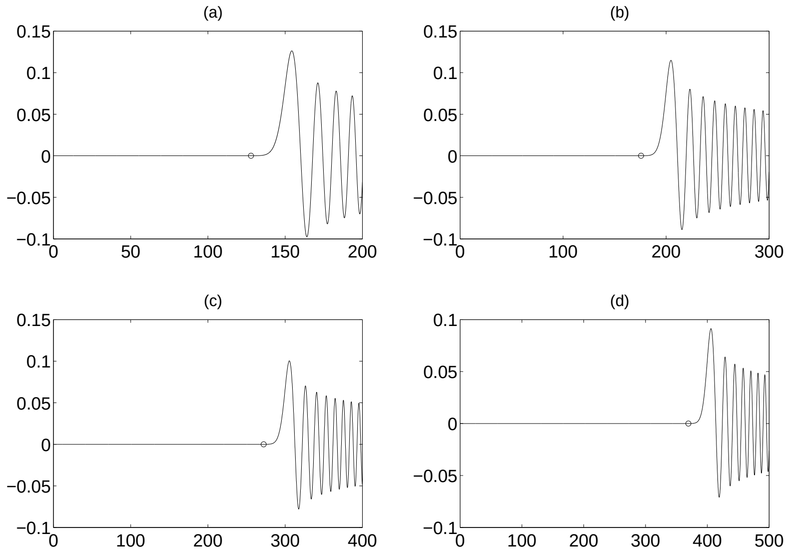

FIG. 3.1. *Bessel function* $J_n(t)$ *for different* n *(circles identify the corresponding points* $n-4.16016n^{\frac{1}{3}}$ *): (a)* $n=150$*; (b)* $n=200$*; (c)* $n=300$*; (d)* $n=400$.

Noticing $e^{2\theta}>1+2\theta$, by the comparison principle for ordinary differential equations, we know that the first negative root of $u_1(\theta)$ is on the right to that of $u_2(\theta)$.

We observe that the root of $u_2(\theta)$ for $\theta<0$ can be found from

$$e^{i\frac{\pi}{3}}\frac{J_{\frac{1}{3}}\left(\frac{n(2\theta)^{\frac{3}{2}}}{3}\right)}{J_{-\frac{1}{3}}\left(\frac{n(2\theta)^{\frac{3}{2}}}{3}\right)}=6^{\frac{1}{3}}\frac{\Gamma\left(\frac{2}{3}\right)}{\Gamma\left(\frac{1}{3}\right)}\cdot\frac{n^{\frac{1}{3}}J_n(n)-\varepsilon}{n^{\frac{2}{3}}J_n'(n)}. \tag{3.12}$$

This is precisely equation (2.5) with $t=\left(\frac{n(-2\theta)^{\frac{3}{2}}}{3}\right)>0$. Therefore a root of equation (3.12) is $-\frac{1}{2}\left(\frac{3t_{n,\varepsilon}}{n}\right)^{\frac{2}{3}}<n^{-\frac{2}{3}}G^*(\varepsilon)$ for $n>\left[\frac{1}{\varepsilon^3}\right]+1$.

This implies that the first negative root of $u_2(\theta)$, and hence that for $u_1(\theta)$, is even bigger. In other words, the biggest $t<n$ at which $J_n(t)$ attains $\frac{\varepsilon}{n^{\frac{1}{3}}}$ is no smaller than

$$n\exp\left(n^{-\frac{2}{3}}G^*(\varepsilon)\right)=n+n^{\frac{1}{3}}G^*(\varepsilon)+o(n^{-\frac{1}{3}}). \tag{3.13}$$

On the other hand, from the series expression

$$\dot{J}_n(t)=\frac{1}{2}\sum_{k=0}^{+\infty}\frac{(-1)^k(n+2k)}{k!(n+k)!}\left(\frac{t}{2}\right)^{n+2k-1}, \tag{3.14}$$

we see that $\dot{J}_n(t)\geq 0$ for t small. Furthermore, it is known that the smallest root of $\dot{J}_n(t)$ is located to the right of $\sqrt{n(n+2)}$ [3]. Accordingly, $\dot{J}_n(t)\geq 0$ on $[0,\sqrt{n(n+2)}]$, hence $J_n(t)$ increases on $[0,n]$. This leads to $0\leq J_n(t)\leq \frac{\varepsilon}{n^{\frac{1}{3}}}$ for $0\leq t\leq n+G^*(\varepsilon)n^{\frac{1}{3}}$. □

For instance, we can take $\varepsilon\approx 10^{-6}$, and corresponding $G^*(\varepsilon)=-4.16016$. Then for $t<n-4.16016n^{\frac{1}{3}}+O\left(\frac{1}{n^{\frac{1}{3}}}\right)$, we have $J_n(t)\approx 0$ for n large enough. Figure 3.1 shows $J_n(t)$ and $n-4.16016n^{\frac{1}{3}}$.

4. Main zone

We consider $F(s,w)=J_{n-k}(t)$ $(0\leq k\leq 30)$ as a function of two variables $s=\frac{k}{n}$ and $w=\frac{t^2}{n^2}-1$.

For n large enough and $t>n-k$, it holds that [2]

$$\begin{aligned}
J_{n-k}(t)&=\sqrt{1-\frac{\arctan\sqrt{w_1}}{\sqrt{w_1}}}\left(\frac{1}{2}J_{\frac{1}{3}}(z)-\frac{\sqrt{3}}{2}Y_{\frac{1}{3}}(z)\right)+O\left((n-k)^{-\frac{4}{3}}\right)\\
&=\frac{\sqrt{3}}{3}\sqrt{\frac{z}{(n-k)\sqrt{w_1}}}(J_{\frac{1}{3}}(z)+J_{-\frac{1}{3}}(z))+O\left((n-k)^{-\frac{4}{3}}\right)\\
&=\frac{\sqrt{3}}{3\sqrt{(n-k)\sqrt{w_1}}}\left[z^{\frac{5}{6}}2^{-\frac{1}{3}}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(4/3+i)}\left(\frac{z^2}{4}\right)^i\right.\\
&\quad\left.+z^{\frac{1}{6}}2^{\frac{1}{3}}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(2/3+i)}\left(\frac{z^2}{4}\right)^i\right]+O\left((n-k)^{-\frac{4}{3}}\right),
\end{aligned}\tag{4.1}$$

where $w_1=\frac{t^2}{(n-k)^2}-1=\frac{w+1}{(1-s)^2}-1$, and z defined in equation (2.21) as $z=(n-k)(\sqrt{w_1}-\arctan\sqrt{w_1})$.

From $n-k=n(1-s)$ and the Taylor series

$$\arctan\sqrt{w_1}=\sqrt{w_1}\sum_{j=0}^{+\infty}\frac{(-1)^j w_1^j}{2j+1},\tag{4.2}$$

we find that

$$\begin{aligned}
&F(s,w)\\
&=\frac{\sqrt{3}}{3}\left[\left(\frac{n(1-s)}{2}\right)^{\frac{1}{3}}x\left(\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{\frac{5}{6}}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(4/3+i)}\left(\frac{n^2(1-s)^2x^3}{4}\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^i\right.\\
&\quad\left.+\left(\frac{n(1-s)}{2}\right)^{-\frac{1}{3}}\left(\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{\frac{1}{6}}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(2/3+i)}\left(\frac{n^2(1-s)^2x^3}{4}\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^i\right]\\
&\quad+O\left((n(1-s))^{-\frac{4}{3}}\right),
\end{aligned}\tag{4.3}$$

with $x=\frac{w-2s+s^2}{(1-s)^2}$.

In a similar way, for n large enough and $t<n-k$, it holds that [2]

$$J_{n-k}(t)=\frac{1}{\pi}\sqrt{1-\frac{\tanh^{-1}\sqrt{-w_1}}{\sqrt{-w_1}}}K_{\frac{1}{3}}((n-k)(\sqrt{-w_1}-\tanh^{-1}\sqrt{-w_1}))+O\left((n-k)^{-\frac{4}{3}}\right). \tag{4.4}$$

It is easy to check this also gives the right-hand side of equation (4.3). So $J_{n-k}(t)$ is expanded as the right-hand side of equation (4.3) uniformly in t.

For a compound function $\Psi(u(x))$, its l-th order derivative may be calculated from

$$\frac{d^l\Psi(u(x))}{dx^l}=\sum_{s=1}^{l}\left[\frac{1}{s!}\frac{d^s\Psi(u)}{du^s}\sum_{\alpha_1+\ldots+\alpha_s=l}\frac{1}{\alpha_1!\cdots\alpha_s!}\cdot\frac{d^{\alpha_1}u}{dx^{\alpha_1}}\cdots\frac{d^{\alpha_s}u}{dx^{\alpha_s}}\right]. \tag{4.5}$$

We may prove the following estimates.

$$\left|\frac{d^l}{dx^l}\left(\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{\frac{5}{6}}\Bigg|_{x=0}\right|\le\left(\frac{1}{3}\right)^{\frac{5}{6}}l!5^l. \tag{4.6}$$

$$\left|\frac{d^l}{dx^l}\left(\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{\frac{1}{6}}\Bigg|_{x=0}\right|\le\left(\frac{1}{3}\right)^{\frac{1}{6}}l!5^l. \tag{4.7}$$

$$\left|\frac{d^l}{dx^l}\left(x^{3i}\left(\frac{1}{2}\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{2i}\right)\Bigg|_{x=0}\right|\le l!\left(\frac{4}{1125}\right)^{i}10^l. \tag{4.8}$$

It then follows

$$\left|\frac{d^l}{dx^l}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(4/3+i)}\left(\frac{n^2(1-s)^2x^3}{4}\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^i\right|$$
$$\le Cl!10^l\sum_{i=0}^{[\frac{l}{3}]}n^{2i}\left(\frac{4e}{1125i}\right)^{2i}\frac{1}{i}\le C(\varepsilon)l!\left(\frac{n^{\frac{1}{3}}}{17\sqrt{|G^*(\varepsilon)|}}\right)^{2l}. \tag{4.9}$$

Here the constant $C(\varepsilon)$ relies on $G^*(\varepsilon)$.

We denote the derivatives of the major part of $F(s,w)$ at $(s,w)=(0,0)$

$$M_{l,m}=\frac{\sqrt{3}}{3l!m!}\frac{\partial^{l+m}}{\partial s^m\partial w^l}\left[\left(\frac{n(1-s)}{2}\right)^{\frac{1}{3}}x\left(\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{\frac{5}{6}}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(4/3+i)}\left(\frac{n^2(1-s)^2x^3}{4}\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^i\right.$$
$$\left.+\left(\frac{n(1-s)}{2}\right)^{-\frac{1}{3}}\left(\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^{\frac{1}{6}}\sum_{i=0}^{+\infty}\frac{(-1)^i}{i!\Gamma(2/3+i)}\left(\frac{n^2(1-s)^2x^3}{4}\sum_{j=0}^{+\infty}\frac{(-x)^j}{2j+3}\right)^i\right]. \tag{4.10}$$

It may be shown that

$$M_{l,m}\le C(\varepsilon)\left(\frac{n^{\frac{1}{3}}}{\sqrt{|G^*(\varepsilon)|}}\right)^{2l+2m+1}. \tag{4.11}$$

Now we are ready to prove Lemma 2.3. For $k=0,\cdots,L$, there exists an integer N, such that if $n\ge N$, $t\in[n-|G^*|n^{\frac{1}{3}},n+|G^*|n^{\frac{1}{3}}]$, it holds that

$$J_{n-k}(t)=\sum_{l=0}^{+\infty}\sum_{m=0}^{+\infty}M_{l,m}\left(\frac{k}{n}\right)^m\left(\frac{t^2}{n^2}-1\right)^l+O((n-k)^{-\frac{4}{3}}). \tag{4.12}$$

Now let $\tilde{a}_k$ $(1\le k\le L)$ satisfy condition (2.3). For n big enough, it holds in the above range of t that $\left|\frac{t^2}{n^2}-1\right|\le\frac{25|G^*(\varepsilon)|}{4n^{\frac{2}{3}}}$. It then follows

$$\begin{aligned}
&\left|\sum_{k=1}^{L}\tilde{a}_kJ_{n-k}(t)-J_n(t)\right|\\
=&\left|\sum_{l=0}^{+\infty}\left(\tilde{a}_1\sum_{m=0}^{+\infty}M_{l,m}\left(\frac{1}{n}\right)^m+\cdots+\tilde{a}_L\sum_{m=0}^{+\infty}M_{l,m}\left(\frac{L}{n}\right)^m-M_{l,0}\right)\left(\frac{t^2}{n^2}-1\right)^l\right|+O\left(n^{-\frac{4}{3}}\right)\\
=&\left|\sum_{l=0}^{+\infty}\sum_{m=4}^{+\infty}M_{l,m}\left(\tilde{a}_1\left(\frac{1}{n}\right)^m+\cdots+\tilde{a}_L\left(\frac{L}{n}\right)^m\right)\left(\frac{t^2}{n^2}-1\right)^l\right|+O\left(n^{-\frac{4}{3}}\right)\\
\le&\left|\sum_{l=0}^{+\infty}\sum_{m=4}^{+\infty}\left(\tilde{a}_1\left(\frac{1}{n}\right)^m+\cdots+\tilde{a}_L\left(\frac{L}{n}\right)^m\right)C\left(\frac{n^{\frac{1}{3}}}{\sqrt{|G^*(\varepsilon)|}}\right)^{2m+2l+1}\left(\frac{t^2}{n^2}-1\right)^l\right|+O\left(n^{-\frac{4}{3}}\right)\\
\le&Cn^{\frac{1}{3}}\sum_{m=1}^{L}|\tilde{a}_k|\left(\frac{mn^{-\frac{1}{3}}}{|G^*(\varepsilon)|}\right)^4+O\left(n^{-\frac{4}{3}}\right)\le\frac{C(\varepsilon)}{n}.
\end{aligned} \tag{4.13}$$

Here $C(\varepsilon)$ depends on ε due to its dependency on $G^*(\varepsilon)$.

5. Transitional zone

In the previous section, we have defined for $0<s=\frac{k}{n}\ll 1$,

$$z(s,w)=n\left(\sqrt{w+2s-s^2}-(1-s)\arctan\frac{\sqrt{w+2s-s^2}}{1-s}\right). \tag{5.1}$$

We claim that

LEMMA 5.1. *For $t\ge n+|G^*(\varepsilon)|n^{\frac{1}{3}}$,*

$$\begin{aligned}
J_{n-k}(t)=\frac{\sqrt{3}}{3}\sqrt{1-\frac{\arctan\sqrt{w}}{\sqrt{w}}}\Big[&J_{\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w})\\
&+J_{-\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w})\Big]+O(n^{-\frac{2}{3}}).
\end{aligned} \tag{5.2}$$

Proof. For $t\ge n+|G^*(\varepsilon)|n^{\frac{1}{3}}$, we may readily show with the Taylor expansion of arctangent function that

$$w\ge 2|G^*(\varepsilon)|n^{-\frac{2}{3}},$$

and

$$n(\sqrt{w}-\arctan\sqrt{w})\ge n\left(\frac{w^{\frac{3}{2}}}{3}-\frac{w^{\frac{5}{2}}}{5}\right)\ge\frac{1}{3}|G^*(\varepsilon)|^{\frac{3}{2}}.$$

As a matter of fact, from the formula

$$\phi(s)=\phi(0)+s\int_0^1 \frac{d\phi(s\eta)}{d\eta}d\eta=\phi(0)+s\frac{d\phi(0)}{d\eta}+s^2\int_0^1(1-\eta)\frac{d^2\phi(s\eta)}{d\eta^2}d\eta, \tag{5.3}$$

we have

$$\begin{aligned} z(s,w)&=n\sqrt{w}-(n-k)\arctan\sqrt{w}+s^2\int_0^1(1-\eta)\frac{n}{\sqrt{w+2s\eta-(s\eta)^2}}d\eta \\ &=n\sqrt{w}-(n-k)\arctan\sqrt{w}+O\left(w^{-\frac{1}{2}}n^{-1}\right). \end{aligned} \tag{5.4}$$

In the same way, we have

$$\sqrt{1-\frac{\arctan\sqrt{w_1}}{\sqrt{w_1}}}=\sqrt{1-\frac{(1-s)\arctan\dfrac{\sqrt{w+2s-s^2}}{1-s}}{\sqrt{w+2s-s^2}}}=\sqrt{1-\frac{\arctan\sqrt{w}}{\sqrt{w}}}+O(w^{-\frac{1}{2}}n^{-1}). \tag{5.5}$$

From the expression [1]

$$J_{\frac{1}{3}}(z)=\frac{\left(\dfrac{z}{2}\right)^{\frac{1}{3}}}{\Gamma\left(\dfrac{1}{2}\right)\Gamma\left(\dfrac{5}{6}\right)}\int_0^\pi \cos(z\cos\theta)\sin^{\frac{2}{3}}\theta d\theta, \tag{5.6}$$

it is easy to get

$$\begin{aligned} \dot{J}_{\frac{1}{3}}(z)=&-\frac{\left(\dfrac{z}{2}\right)^{\frac{1}{3}}}{\Gamma\left(\dfrac{1}{2}\right)\Gamma\left(\dfrac{5}{6}\right)}\int_0^\pi \sin(z\cos\theta)\cos\theta\sin^{\frac{2}{3}}\theta d\theta \\ &+\frac{\dfrac{1}{6}\left(\dfrac{z}{2}\right)^{-\frac{2}{3}}}{\Gamma\left(\dfrac{1}{2}\right)\Gamma\left(\dfrac{5}{6}\right)}\int_0^\pi \cos(z\cos\theta)\sin^{\frac{2}{3}}\theta d\theta. \end{aligned} \tag{5.7}$$

Together with equations (5.3) and (5.4), one has

$$\begin{aligned} J_{\frac{1}{3}}(z(s,w))=&J_{\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w}) \\ &+\int_0^1 \dot{J}_{\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w}+O(\frac{1}{\sqrt{wn}})\eta)(O(\frac{1}{\sqrt{wn}}))d\eta \\ =&J_{\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w})+O\left(\frac{(\sqrt{w}-\arctan\sqrt{w})^{\frac{1}{3}}}{n^{\frac{2}{3}}\sqrt{w}}\right). \end{aligned} \tag{5.8}$$

In the same way, we have

$$J_{-\frac{1}{3}}(z(s,w))=J_{-\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w})+O\left(\frac{(\sqrt{w}-\arctan\sqrt{w})^{\frac{1}{3}}}{n^{\frac{2}{3}}\sqrt{w}}\right). \tag{5.9}$$

Now from equations (4.1), (5.5), (5.8) and (5.9), we complete the proof of equation (5.2) with

$$J_{n-k}(t)=\frac{\sqrt{3}}{3}\Big(J_{\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w})+J_{-\frac{1}{3}}(n\sqrt{w}-(n-k)\arctan\sqrt{w})\Big)\cdot \left(\sqrt{1-\frac{\arctan\sqrt{w}}{\sqrt{w}}}+O\left(\frac{1}{\sqrt{wn}}\right)\right)+O\left(\frac{(\sqrt{w}-\arctan\sqrt{w})^{\frac{1}{3}}}{n^{\frac{2}{3}}\sqrt{w}}\right). \tag{5.10}$$

∎

Then let us return to prove Lemma 2.4.

Proof. Taking $z_k=n\sqrt{w}-n\arctan\sqrt{w}+k\arctan\sqrt{w}$, for n large enough and $t\in[n+|G^*(\varepsilon)|n^{\frac{1}{3}},n+n^{\frac{1}{2}}]$, one has

$$\frac{2|G^*(\varepsilon)|}{n^{\frac{2}{3}}}\le w\le\frac{2}{n^{\frac{1}{2}}}, \tag{5.11}$$

and

$$\delta\equiv\frac{|G^*(\varepsilon)|^{\frac{3}{2}}}{3}\le z_k\le n^{\frac{1}{4}}. \tag{5.12}$$

On the other hand, it holds that

$$\begin{aligned}&J_{\frac{1}{3}}(z_k)\\ =&\sum_{l=0}^{3}\frac{J_{\frac{1}{3}}^{(l)}(n\sqrt{w}-n\arctan\sqrt{w})}{l!}(k\arctan\sqrt{w})^l\\ &+\frac{(k\arctan\sqrt{w})^4}{3!}\int_0^1(1-t)^3J_{\frac{1}{3}}^{(4)}(n\sqrt{w}-n\arctan\sqrt{w}+tk\arctan\sqrt{w})dt\\ \equiv&\sum_{l=0}^{3}\frac{J_{\frac{1}{3}}^{(l)}(n\sqrt{w}-n\arctan\sqrt{w})}{l!}(k\arctan\sqrt{w})^l+R_k(t).\end{aligned} \tag{5.13}$$

Further differentiation of equation (5.7) gives

$$J_{\frac{1}{3}}^{(l)}(x)=\frac{2^{-\frac{1}{3}}}{\Gamma\left(-\frac{1}{3}\right)\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{5}{6}\right)}\sum_{m=0}^{l}\Bigg[C_l^m\frac{(-1)^m\Gamma(m-\frac{1}{3})}{x^{m-\frac{1}{3}}}\cdot \int_0^\pi\cos\left(x\cos\theta+\frac{(l-m)\pi}{2}\right)(\cos\theta)^{l-m}\sin^{\frac{2}{3}}\theta d\theta\Bigg]. \tag{5.14}$$

Accordingly, it holds that

$$|J_{\frac{1}{3}}^{(l)}(x)|\le Cl!x^{\frac{1}{3}}\sum_{m=0}^{l}C_l^m\frac{1}{x^m}=Cl!x^{\frac{1}{3}}\left(\frac{1+x}{x}\right)^l. \tag{5.15}$$

From inequalities (5.12) and (5.15), we find the remainder in equation (5.13)

$$|R_k(t)|\le Cn^{\frac{1}{12}}\left(k\arctan\sqrt{w}\left(1+\frac{1}{\delta}\right)\right)^4. \tag{5.16}$$

It further holds that

$$\begin{aligned}
&\left|\sum_{k=1}^{L}\tilde{a}_k J_{\frac{1}{3}}(z_k)-J_{\frac{1}{3}}(z_0)\right|\\
=&\left|\sum_{k=1}^{L}\tilde{a}_k\left(\sum_{l=0}^{3}\frac{J_{\frac{1}{3}}^{(l)}(z_0)}{l!}(k\arctan\sqrt{w})^l+R_k(t)\right)-J_{\frac{1}{3}}(z_0)\right|\\
\le&\left|\sum_{l=0}^{3}\frac{J_{\frac{1}{3}}^{(l)}(z_0)}{l!}(\arctan\sqrt{w})^l\left(\sum_{k=1}^{L}\tilde{a}_k k^l-\delta_{l,0}\right)\right|+\sum_{k=1}^{L}|\tilde{a}_k R_k|\\
\le&Cn^{\frac{1}{12}}\left(\frac{\left(1+\frac{1}{\delta}\right)}{n^{\frac{1}{4}}}\right)^4\sum_{k=1}^{L}|\tilde{a}_k|\le\frac{C(\varepsilon)}{n^{\frac{11}{12}}}.
\end{aligned}\tag{5.17}$$

Together with equation (5.2), for $t\in[n+|G^*(\varepsilon)|n^{\frac{1}{3}},n+n^{\frac{1}{2}}]$ one has,

$$\left|\sum_{k=1}^{L}\tilde{a}_k J_{n-k}(t)-J_{n-k}(t)\right|\le\frac{C(\varepsilon)}{n^{\frac{7}{6}}}.\tag{5.18}$$

This completes the proof. ∎

6. Asymptotic zone

Now we prove Lemma 2.5.

Proof. In fact, direct calculation shows

$$\begin{aligned}
&z^{\frac{1}{3}}\int_0^{\pi}\cos(z\cos\theta)\sin^{\frac{2}{3}}\theta d\theta\\
=&2z^{\frac{1}{3}}\int_0^1\cos(-z+zt^6)6t^4\left(\frac{1}{\sqrt[6]{2}}+t\int_0^1\frac{r^5t^5}{(2-r^6t^6)^{\frac{7}{6}}}dr\right)dt\\
=&\frac{2z^{\frac{1}{3}}}{\sqrt[6]{2}}\int_0^1\frac{\cos(-z+zt)}{t^{\frac{1}{6}}}dt+O\left(z^{-\frac{2}{3}}\right)\\
=&\frac{\pi\cos z}{2^{\frac{1}{6}}\Gamma\left(\frac{1}{6}\right)\cos\left(\frac{\pi}{12}\right)z^{\frac{1}{2}}}+\frac{\pi\sin z}{2^{\frac{1}{6}}\Gamma\left(\frac{1}{6}\right)\sin\left(\frac{\pi}{12}\right)z^{\frac{1}{2}}}+o\left(z^{-\frac{1}{2}}\right).
\end{aligned}\tag{6.1}$$

This gives

$$J_{\frac{1}{3}}(z)=\frac{\sqrt{\pi}\cos z}{2^{\frac{1}{2}}\Gamma\left(\frac{5}{6}\right)\Gamma\left(\frac{1}{6}\right)\cos\left(\frac{\pi}{12}\right)z^{\frac{1}{2}}}+\frac{\sqrt{\pi}\sin z}{2^{\frac{1}{2}}\Gamma\left(\frac{5}{6}\right)\Gamma\left(\frac{1}{6}\right)\sin\left(\frac{\pi}{12}\right)z^{\frac{1}{2}}}+o\left(z^{-\frac{1}{2}}\right).\tag{6.2}$$

In the same way, we have

$$J_{-\frac{1}{3}}(z)=\frac{\sqrt{\pi}\cos z}{2^{\frac{1}{2}}\Gamma\left(\frac{5}{6}\right)\Gamma\left(\frac{1}{6}\right)\cos\left(\frac{5\pi}{12}\right)z^{\frac{1}{2}}}+\frac{\sqrt{\pi}\sin z}{2^{\frac{1}{2}}\Gamma\left(\frac{5}{6}\right)\Gamma\left(\frac{1}{6}\right)\sin\left(\frac{5\pi}{12}\right)z^{\frac{1}{2}}}+o\left(z^{-\frac{1}{2}}\right).\tag{6.3}$$

If $t\in\left[n+n^{\frac{1}{2}},n\sqrt{1+A_1}\right]$, then $\frac{1}{n^{\frac{1}{2}}}\leq\frac{t^2}{n^2}-1\leq A_1$. On the other hand, recall that

$$z(s,w)=n\sqrt{\frac{t^2}{n^2}-1}-n\arctan\sqrt{\frac{t^2}{n^2}-1}+k\sqrt{\frac{t^2}{n^2}-1}+O\left(n^{-\frac{5}{6}}\right). \tag{6.4}$$

From equations (6.2), (6.3) and (4.1), one has

$$\begin{aligned}
&J_{n-k}(t)\\
=&\sqrt{1-\frac{\arctan\sqrt{w}}{\sqrt{w}}}\frac{\sqrt{\pi}\left(\sin\frac{\pi}{12}+\cos\frac{\pi}{12}\right)}{\sqrt{3}\Gamma\left(\frac{5}{6}\right)\Gamma\left(\frac{1}{6}\right)\sin\left(\frac{\pi}{12}\right)\cos\left(\frac{\pi}{12}\right)}\cdot\\
&\left(\frac{\cos(z-\frac{\pi}{4})}{z^{\frac{1}{2}}}+o\left(\frac{1}{z^{\frac{1}{2}}}\right)\right)+O\left(n^{-\frac{4}{3}}\right)\\
\equiv&\sqrt{\frac{2}{\pi}\left(1-\frac{2\arctan\sqrt{w}}{\sqrt{w}}\right)}\left[\frac{\cos(n\sqrt{w}-(n-k)\arctan\sqrt{w}-\frac{\pi}{4})}{(n\sqrt{w}-n\arctan\sqrt{w})^{\frac{1}{2}}}\right.\\
&\left.+\frac{R_{n,k}(t)}{(n\sqrt{w}-n\arctan\sqrt{w})^{\frac{1}{2}}}\right].
\end{aligned} \tag{6.5}$$

With n big enough, we may set

$$|R_{n,k}|(t)<\varepsilon. \tag{6.6}$$

□

Now we are ready to prove a more accurate estimate in Lemma 2.6.

Proof. With $\tilde{a}_k$ satisfying conditions (2.3), (2.14)-(2.17), we define

$$E(\theta)=\sum_{k=1}^{30}\tilde{a}_k\cos k\theta-1. \tag{6.7}$$

Direct calculation shows that at $\theta=1.30732057$, $|E(\theta)|$ attains its maximum of 0.00149822. Namely, we have on $[0,\pi/2]$,

$$\left|\sum_{k=1}^{30}\tilde{a}_k\cos k\theta-1\right|\leq 0.00149822. \tag{6.8}$$

In the same way, we have on $[0,\pi/2]$,

$$\left|\sum_{k=1}^{30}\tilde{a}_k\sin k\theta\right|\leq 0.00244607. \tag{6.9}$$

We denote a phase

$$\Phi=n\sqrt{w}-n\arctan\sqrt{w}-\frac{\pi}{4}. \tag{6.10}$$

From equation (2.9) and inequalities (6.8) and (6.9), for N large enough and $n\geq N$, $t\in[n+n^{\frac{1}{2}},n\sqrt{1+A_1}]$, one has

$$\left|\sum_{k=1}^{30}\tilde{a}_kJ_{n-k}(t)-J_n(t)\right|$$

$$=\sqrt{\frac{2}{\pi}}\frac{1}{(t^2-n^2)^{\frac{1}{4}}}\left|\sum_{k=1}^{30}\tilde{a}_k\left(\cos\left(\Phi+k\arctan\sqrt{w}\right)+R_{n,k}(t)\right)-\cos\Phi-R_{n,0}(t)\right|$$
$$\leq\sqrt{\frac{2}{\pi}}\frac{1}{(t^2-n^2)^{\frac{1}{4}}}\left\{\left|\sum_{k=1}^{30}\tilde{a}_k\cos\left(k\arctan\sqrt{w}\right)-1\right|\right.$$
$$\left.+\left|\sum_{k=1}^{30}\tilde{a}_k\sin\left(k\arctan\sqrt{w}\right)\right|+\sum_{k=1}^{30}|\tilde{a}_kR_{n,k}(t)|+|R_{n,0}(t)|\right\}$$
$$\leq\sqrt{\frac{2}{\pi}}\frac{1}{(t^2-n^2)^{\frac{1}{4}}}(0.00394429+\varepsilon). \tag{6.11}$$

Finally we prove Lemma 2.7. □

Proof. For n large enough and fixed k, when $t\geq n\sqrt{1+A_1}$ with A_1 defined in equation (2.18), we know that [1]

$$J_{n-k}(t)=\sqrt{\frac{2}{\pi n(\sqrt{w}-\arctan\sqrt{w})}}\cos\left(n\sqrt{w}-(n-k)\arctan\sqrt{w}-\frac{\pi}{4}\right)+O\left(\frac{1}{z^{\frac{3}{2}}}\right). \tag{6.12}$$

For $t\geq n\sqrt{1+A_1}$, noticing $\arctan\sqrt{\frac{t^2}{n^2}-1}=\frac{\pi}{2}-\arctan\left(\sqrt{\frac{t^2}{n^2}-1}\right)^{-1}$, and taking $\Phi=n\sqrt{w}-n\arctan\sqrt{w}-\frac{\pi}{4}$, we have

$$J_{n-k}(t)=\sqrt{\frac{2}{\pi\left(n\sqrt{w}-n\arctan\sqrt{w}\right)}}\cos\left(\Phi-k\arctan\frac{1}{\sqrt{w}}+\frac{k\pi}{2}\right)+O\left(z^{-\frac{3}{2}}\right). \tag{6.13}$$

This gives

$$J_{n-k}(t)$$
$$=\sqrt{\frac{2}{\pi\left(n\sqrt{w}-n\arctan\sqrt{w}\right)}}\cos\left(\Phi-k\arctan\frac{1}{\sqrt{w}}+\frac{k\pi}{2}\right)+O\left(z^{-\frac{3}{2}}\right).$$
$$=\sqrt{\frac{2}{\pi\left(n\sqrt{w}-n\arctan\sqrt{w}\right)}}\left\{\cos\Phi\sum_{l=0}^{3}\cos\left(\frac{k\pi}{2}+\frac{l\pi}{2}\right)\frac{\left(-k\arctan\frac{1}{\sqrt{w}}\right)^l}{l!}\right.$$
$$-\sin\Phi\sum_{l=0}^{3}\sin\left(\frac{k\pi}{2}+\frac{l\pi}{2}\right)\frac{\left(-k\arctan\frac{1}{\sqrt{w}}\right)^l}{l!}$$
$$+\cos\Phi\cos\left(\frac{k\pi}{2}+\frac{l\pi}{2}+\xi_1(t)\right)\frac{\left(-k\arctan\frac{1}{\sqrt{w}}\right)^4}{4!}$$
$$\left.+\sin\Phi\sin\left(\frac{k\pi}{2}+\frac{l\pi}{2}+\xi_2(t)\right)\frac{\left(-k\arctan\frac{1}{\sqrt{w}}\right)^4}{4!}\right\}+O\left(z^{-\frac{3}{2}}\right). \tag{6.14}$$

Therefore, there exists an integer N such that, for $n>N$, it holds that

$$\begin{aligned}
&\left|\sum_{k=1}^{30}\tilde{a}_k J_{n-k}(t)-J_n(t)\right| \\
\leq&\left|\sqrt{\frac{2}{\pi\left(n\sqrt{w}-n\arctan\sqrt{w}\right)}}\cos\Phi\sum_{k=1}^{30}\tilde{a}_k\cos\left(\frac{k\pi}{2}+\frac{l\pi}{2}+\xi_1(t)\right)\frac{(-k\arctan\frac{1}{\sqrt{w}})^4}{4!}\right| \\
&+\left|\sqrt{\frac{2}{\pi\left(n\sqrt{w}-n\arctan\sqrt{w}\right)}}\sin\Phi\sum_{k=1}^{30}\tilde{a}_k\sin\left(\frac{k\pi}{2}+\frac{l\pi}{2}+\xi_2(t)\right)\frac{(-k\arctan\frac{1}{\sqrt{w}})^4}{4!}\right| \\
&+O\left(z^{-\frac{3}{2}}\right) \\
\leq&2A\sqrt{\frac{2}{\pi\left(n\sqrt{w}-n\arctan\sqrt{w}\right)}}\left(15\arctan\frac{1}{\sqrt{w}}\right)^4+O\left(z^{-\frac{3}{2}}\right).
\end{aligned}\tag{6.15}$$

This completes the proof. □

7. ALmost EXact boundary condition for harmonic chain

We consider a rescaled semi-infinite harmonic chain with displacement $u_n(t)$ for $n\in\mathbb{N}$, governed by Newton's law

$$\begin{aligned}
&\ddot{u}_n(t)=u_{n-1}(t)-2u_n(t)+u_{n+1}(t),\\
&u_n(0)=0,\quad \dot{u}_n(0)=0.
\end{aligned}\tag{7.1}$$

The displacement $u_0(t)$ is a given function. It may be readily shown [7] that

$$u_n(t)=u_0(t)*\frac{2nJ_{2n}(2t)}{t},\tag{7.2}$$

where "$*$" stands for convolution. We denote the kernel function as

$$g_n(t)=\frac{2nJ_{2n}(2t)}{t}.\tag{7.3}$$

From the main theorem, we make use of the recursive relation for the derivatives of Bessel functions to obtain the following result.

LEMMA 7.1. *There exists a set of numbers a_k, b_k for $k=1,\cdots,15$ such that for any given small $\varepsilon>0$, there exists an integer N such that, for $n>N$ and $t\in[0,+\infty)$, it holds that*

$$\left|\sum_{k=1}^{15}a_k g_{n-k}(t)+\sum_{k=1}^{15}b_k\dot{g}_{n-k}(t)-g_n(t)\right|<\frac{\varepsilon}{n^{\frac{1}{3}}}.\tag{7.4}$$

The coefficients may be obtained as follows.

k	a_k	b_k
1	−109.6025083485	−14.7037545028
2	−2097.7449276669	−565.8956925015
3	−16397.2434307511	−6987.0154168434
4	−67599.3626830461	−42745.1519585622
5	−162239.5589866582	−154522.0935326181
6	−226809.2228360120	−360718.1501167417

7	−148864.1935697496	−570137.5721903182
8	54082.5525551020	−624080.7335295006
9	209470.0946578346	−475111.0133192166
10	206148.6740564536	−248307.6661901102
11	111712.8002405539	−86134.1925588502
12	35725.8382042134	−18584.6750406846
13	6413.0325582591	−2205.0724859373
14	550.2656303204	−110.3881561666
15	14.6710381195	−0.9974265280

For instance, with $n=100$ we compare the kernel function $g_n(t)$ with the linear combination $\sum_{k=1}^{15}(a_k g_{n-k}(t)+b_k\dot{g}_{n-k}(t))$ in Figure 7.1. They coincide very well. The difference is on the order of 10^{-4}.

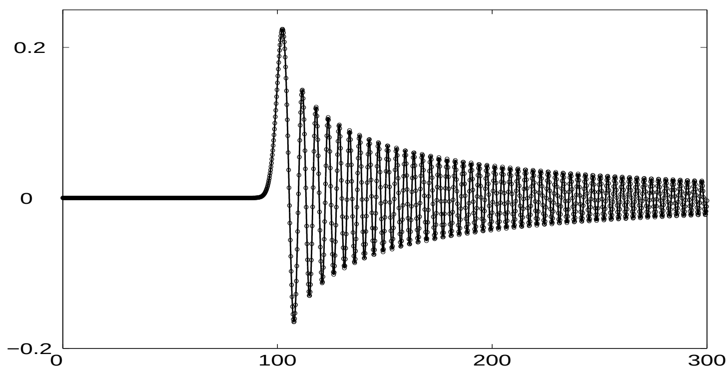

FIG. 7.1. *Comparison of* $g_{100}(t)$ *(solid line) and* $\sum_{k=1}^{15}(a_k g_{100-k}(t)+b_k\dot{g}_{100-k}(t))$ *(circles).*

Other results about the approximation are the same as Lemma 2.6 and Lemma 2.7. For n large enough $\left|\sum_{k=1}^{15}\tilde{a}_k g_{n-k}(t)+\sum_{k=1}^{15}\tilde{b}_k\dot{g}_{n-k}(t)-g_n(t)\right|$ is not only smaller than $\frac{\varepsilon}{n^{\frac{1}{3}}}$ over the entire time axis, but also is much smaller than that for $g_n(t)$'s leading term on every zone.

This result naturally leads to a boundary condition, which turns out to be very accurate. Suppose we perform numerical simulation of the semi-infinite chain over a finite segment with $1\le n\le J$ only. We formulate an ALEX (ALmost EXact) boundary condition as follows.

$$u_J(t)=\sum_{k=1}^{15}a_k u_{J-k}(t)+\sum_{k=1}^{15}b_k\dot{u}_{J-k}(t). \tag{7.5}$$

With this boundary condition, we calculate the reflection coefficient by plugging the Fourier mode $e^{i\omega t-i\xi p}+R(\xi)e^{i\omega t+i\xi p}$ into the boundary condition. Here $\xi\in[0,\pi]$ is the wave number, and $\omega = 2\sin\frac{\xi}{2}$ is the frequency. We find that

$$|R(\xi)| = \left| \frac{1 - \sum_{k=1}^{15} (a_k e^{ik\xi} + i\omega b_k e^{ik\xi})}{1 - \sum_{k=1}^{15} (a_k e^{-ik\xi} + i\omega b_k e^{-ik\xi})} \right|. \tag{7.6}$$

As shown in Figure 7.2, the reflection coefficient is on the order of 10^{-9} for wave numbers up to $\pi/2$, indicating the extraordinary ability of the ALEX boundary condition in suppressing spurious reflections. We remark that the time history kernel convolution is an exact boundary condition, for which the reflection should be zero theoretically. However, the temporal discretization and round-off error may induce some minor reflections.

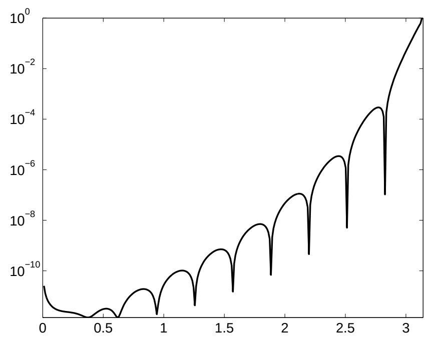

FIG. 7.2. *Reflection coefficient $|R(k)|$ as a function of the wave number k.*

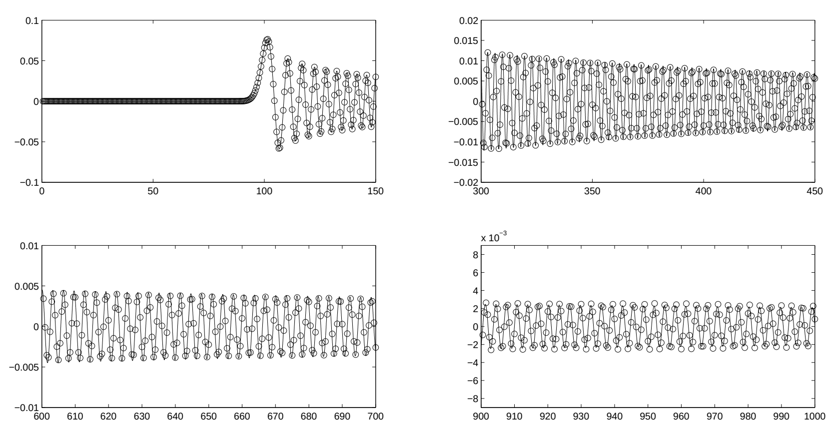

FIG. 7.3. *Simulation of the harmonic lattice with ALEX boundary condition: $u_{99}^{ex}(t)$ (solid line) and $u_{99}(t)$ (circles) on time intervals [0,150], [300,450], [600,700], and [900,1000], respectively.*

To resolve the harmonic chain (7.1), we use the central difference scheme

$$\begin{aligned}\frac{u_n^{l+1}-2u_n^l+u_n^{l-1}}{\triangle t^2}=&\frac{1}{4}(u_{n+1}^{l+1}-2u_n^{l+1}+u_{n-1}^{l+1})+\frac{1}{2}(u_{n+1}^l-2u_n^l+u_{n-1}^l)\\&+\frac{1}{4}(u_{n+1}^{l-1}-2u_n^{l-1}+u_{n-1}^{l-1}),\end{aligned}\tag{7.7}$$

for $1\le n\le J-2$ and $l\ge 1$. For $n=J-1$, we take

$$\begin{aligned}\frac{u_{J-1}^{l+1}-2u_{J-1}^l+u_{J-1}^{l-1}}{\triangle t^2}=&\frac{1}{4}(u_J^l-2u_{J-1}^{l+1}+u_{J-2}^{l+1})+\frac{1}{2}(u_J^l-2u_{J-1}^l+u_{J-2}^l)\\&+\frac{1}{4}(u_J^l-2u_{J-1}^{l-1}+u_{J-2}^{l-1}).\end{aligned}\tag{7.8}$$

Moreover, as the scheme requires initial data at both the t^0 and t^1 level, the data at the t^1 level is prepared with a much smaller time step size to maintain the accuracy.

The boundary condition reads

$$u_J^l=\sum_{k=1}^{15}a_k\left(\frac{1}{4}u_{J-k}^{l+1}+\frac{1}{2}u_{J-k}^l+\frac{1}{4}u_{J-k}^{l-1}\right)+\sum_{k=1}^{15}b_k\frac{u_{J-k}^{l+1}-u_{J-k}^{l-1}}{2\triangle t}.\tag{7.9}$$

With $u_0(t)=\sin 3t$, $\triangle t=0.005$ and $J=100$, the exact solution $u_{99}^{ex}(t)$ calculated with a much extended computational domain, and our numerical result $u_{99}(t)$ are displayed in Figure 7.3 for comparison. There appears no observable difference, demonstrating the high accuracy of the ALEX boundary condition.

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