Quantum networks: Anti-core of spin chains

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Abstract

The purpose of this paper is to exhibit a quantum network phenomenon—the anti-core—that goes against the classical network concept of congestion core. Classical networks idealized as infinite, Gromov hyperbolic spaces with least-cost path routing (and subject to a technical condition on the Gromov boundary) have a congestion core, defined as a subnetwork that routing paths have a high probability of visiting. Here, we consider quantum networks, more specifically spin chains, define the so-called maximum excitation transfer probability $p_{\max}(i,j)$ between spin i and spin j, and show that the central spin has among all other spins the lowest probability of being excited or transmitting its excitation. The anti-core is singled out by analytical formulas for $p_{\max}(i,j)$, revealing the number theoretic properties of quantum chains. By engineering the chain, we further show that this probability can be made vanishingly small.

1 Introduction

Probably the most significant result of the Gromov analysis of classical networks [4, 6] is existence of a congestion core. Under a network protocol that sends the packets along least cost paths, the *core* can be qualitatively defined as a point where most of the geodesics (least cost paths) converge, creating packet drops, high retransmission rates, and other nuisances under the TCP-IP protocol [10]. Existence of the core has been experimentally observed [11] and mathematically proved [8] if the network is Gromov hyperbolic, subject to some highly technical conditions related to the Gromov boundary [2]. A Gromov hyperbolic network can intuitively be defined as a network that "looks like" a negatively curved Riemannian manifold (e.g., a saddle) when viewed from a distance. See, e.g., [3] for a precise definition.

Next to classical networks, one can envision quantum networks: the nodes are spins that can be up $|\uparrow\rangle$ (not excited) or down $|\downarrow\rangle$ (excited) and the links are quantum mechanical couplings of the XX or Heisenberg type. Given some random source-destination pair (i,j), a valid question is whether some spin ω could act as a "core," that is, a spin that could be excited no matter what the source and the destination are. For a linear chain, one would expect such a congestion core in the center as classically any excitation in one half of the chain would have to transit the center of the chain to reach the other half. In this work, we demonstrate that quantum-mechanically the transmission of excitations does not need to occur this way, and in fact the center ω of an odd-length spin chain can act as an "anti-core," excitation of which is avoided.

This "anti-core," or "anti-gravity" center as it was originally called, was first observed in [7]. The anti-core ω was defined as a point of high inertia, $\sum_i d^\alpha(i,\omega)$, $\alpha \geq 1$, as opposed to the classical congestion core that has minimum inertia owing to the negative curvature of the underlying space [9, Theorem 3.2.1]. The inertia quantifies how difficult communication to and from the anti-core is.

As it has been done along this line of work, a pre-metric $d(\cdot,\cdot)$ based on the *Information Transfer Capacity (ITC)* (see Sec. 2) is employed. Unlike standard quantum mechanical distances [13, 15], [12, pages 412-413], this "distance" measure aims to quantify not how distant two fixed quantum states are, but how close to a desired target state a quantum state can get under the evolution of a particular Hamiltonian. The initial and target states are typically orthogonal.

In this paper, we provide an *analytical* justification of the numerically observed anti-core phenomenon in spin chains with XX coupling, starting with finite-length chains, extending the ITC concept to semi- and bi-infinite cases (Sec. 3), and finally *proving* that $d(\omega, j) \geq d(i,j)$, $\forall j \neq \omega$ in Sec. 4. We further show that by adding a bias on the central spin its *"anti-core"* property can be made stronger in the sense that the probability of transmission of the excitation to and from it is infinitesimally small (Sec. 5).

The remaining nagging question is why was it observed in [7] that spin chains appear Gromov-hyperbolic and have an anti-core, while classical networks are Gromov hyperbolic with the opposite core? This will be clarified in Sec. 5 by means of a spin chain example, showing that its Gromov boundary has *only one* point, while classical networks need to have *at least two points* in their Gromov boundary for the core to emerge.

2 Metrization of homogeneous spin chains

We consider a linear array of two-level systems (spin $\frac{1}{2}$ particles) with uniform coupling between adjacent spins (homogeneous spin chain) made up of an odd number N of physically equally spaced spins with coupling Hamiltonian

$$H = \sum_{i=1}^{N-1} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \epsilon \sigma_i^z \sigma_{i+1}^z \right).$$

Here we shall be primarily interested in the case of XX coupling, for which $\epsilon = 0$. The factor $\sigma_i^{x,y,z}$ is the Pauli matrix along the x, y, or z direction of spin i in the array, i.e.,

$$\sigma_i^{x,y,z} = I_{2\times 2} \otimes \ldots \otimes I_{2\times 2} \otimes \sigma^{x,y,z} \otimes I_{2\times 2} \otimes \ldots \otimes I_{2\times 2},$$

	λ_k	v_{kj}
XX coupling ($\epsilon = 0$)	$2\cos\frac{\pi k}{N+1}$	$\sqrt{\frac{2}{N+1}}\sin\frac{\pi jk}{N+1}$

Table 1: Eigenvalues and eigenvectors of Single Excitation Subspace Hamiltonian H_1 under XX coupling [14].

where the factor $\sigma^{x,y,z}$ occupies the ith position among the N factors and $\sigma^{x,y,z}$ is one of the single spin Pauli operators

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

It is easily seen that H is *real* and symmetric.

2.1 Single excitation subspace

The $2^N \times 2^N$ Hamiltonian commutes with the operator $S = \sum_{i=1}^N \sigma_i^z$ which counts the total number of excitations. The Hilbert space can therefore be decomposed into subspaces corresponding to the number of excitations. Define $|i\rangle = |\uparrow \cdots \uparrow\downarrow\uparrow \cdots \uparrow\rangle$ to be the quantum state in which the excitation is on spin i. The single excitation subspace $\mathcal{H}_1$ is spanned by $\{|i\rangle : i = 1, \ldots, N\}$. Restricted to this subspace, the Hamiltonian in this natural basis takes the form

$$H_1 = \begin{pmatrix}
\epsilon & 1 & \dots & 0 & 0 & 0 & \dots & 0 & 0 \\
1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots \\
0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 \\
0 & 0 & \dots & 1 & 0 & 1 & \dots & 0 & 0 \\
0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 \\
\vdots & \vdots & & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 1 \\
0 & 0 & \dots & 0 & 0 & 0 & \dots & 1 & \epsilon
\end{pmatrix}.$$

For XX coupling ($\epsilon = 0$), H_1 becomes the $N \times N$ Toeplitz matrix T_N made up of zeros on the diagonal, ones on the super- and subdiagonal and zeros everywhere else. Table 1 shows the eigenvalues and eigenvectors of H_1.

2.2 Information Transfer Capacity (ITC) semi-metric

The probability for the system to transfer from state $|i\rangle$ to state $|j\rangle$ in an amount of time t, that is, the probability of transfer of the excitation from spin i to spin

j in an amount of time t, is

$$p_t(i,j) = |\langle i|e^{-\imath H_1 t}|j\rangle|^2.$$

Observe that $\sum_{j=1}^{N} p_t(i,j) = 1$. In order to remove the dependency of the probability distribution on the time, we proceed as in Refs [5, 7]:

$$p_t(i,j) = \left|\sum_{k=1}^{N} e^{-\imath\lambda_k t}\langle i|v_k\rangle\langle v_k|j\rangle\right|^2 \tag{1a}$$

$$\leq \left|\sum_{k=1}^{N} |\langle i|v_k\rangle\langle v_k|j\rangle|\right|^2 =: p_{\max}(i,j). \tag{1b}$$

We refer to $p_{\max}(i,j)$ as *maximum transfer probability* from $|i\rangle$ to $|j\rangle$ or *Information Transfer Capacity (ITC)* between $|i\rangle$ and $|j\rangle$. Its explicit formulation for XX chains is easily obtained from (1) and Table 1:

$$\sqrt{p_{\max}(i,j)} = \frac{2}{N+1}\sum_{k=1}^{2n+1}\left|\sin\frac{\pi k i}{2(n+1)}\right|\left|\sin\frac{\pi k j}{2(n+1)}\right|. \tag{2}$$

Lemma 1 *$p_{\max}(i,j) \leq 1$ and $p_{\max}(i,i) = 1$ for all $i,j = 1,\ldots,N$.*

Proof. $p_{\max}(i,i) = 1$ follows directly from (1a), setting $i = j$ and $t = 0$ and noting that the eigenvectors $|v_m\rangle$ form an orthonormal basis. $p_{\max}(i,j) \leq 1$ then follows from a Cauchy-Schwartz argument. ■

The preceding lemma tells us that in order to define a (pre)metric from $p_{\max}(i,j)$, it is legitimate to take the log and define

$$d(i,j) := -\log p_{\max}(i,j) \tag{3}$$

on the single excitation subspace of the chain. From Lemma 1, $d(i,i) = 0$ and $d(i,j) \geq 0$, and clearly $d(i,j) = d(j,i)$. Observe, however, that $d(i,j)$ can vanish for $i \neq j$ and the triangle inequality need not be satisfied, so that $d(i,j)$ is just a pre-metric, but this will be sufficient for our purposes.

The definition of $d(i,j)$ bears some commonality with sensor networks [1], where the Packet Reception Rate $\mathrm{PRR}(i,j)$ from sensor i to sensor j—that is, the probability of successful transmission of packets from i to j—defines a premetric $d(i,j) = -\log \mathrm{PRR}(i,j)$.

3 Infinite chains

In this section, we develop some asymptotic formulas for $\sqrt{p_{\max}(i,j)}$ for infinite-length chains in order to show that the central spin $n+1$ of a chain of odd length $N = 2n+1$ has the lowest probability of being excited, hence justifying the terminology of "anti-core," even for $N \to \infty$. This will further reveal a classical-quantum discrepancy: Classical dynamical systems interconnected in an homogeneous infinite chain architecture exhibit the so-called *shift-invariance,* that is, those dynamical interactions depending on the positions i and j of two systems in the chain in fact depend only on the distance $|i-j|$. As a corollary of the asymptotic formulas, this well known shift-invariance does not carry over to the quantum chains—no matter how the chain is extended to infinity, two spins in their transfer probability interaction keep properties specific to some number theoretic properties of their positions i and j. Moreover, in a classical chain, the interaction at infinity is insensitive to the way the limit is taken: either the chain starts at a specific system, say 1, and extends to infinity as

$$(1,2,3,...), \quad (\text{"semi-infinite chain," written } \rightarrow)$$

or the chain starts at its center ω and extends both ways as

$$(...,\omega-2,\omega-1,\omega,\omega+1,\omega+2,...), \quad (\text{"doubly-infinite chain" written } \leftrightarrow).$$

It is another quantum mechanical effect that the two infinite chains do not yield the same asymptotic transfer probabilities.

3.1 Semi-infinite chains

Theorem 1 *For a semi-infinite XX chain, the maximum transition probabilities are given by*

$$\begin{aligned}\sqrt{p^{\rightarrow}_{\max}(i,j)} &= \frac{4}{\pi^2}\left(2+\sum_{m=2,4,\ldots}\frac{4}{(m^2\mathbf{j}^2-1)(m^2\mathbf{i}^2-1)}\right)\\ &= \frac{8}{\pi^2}\left(\frac{\mathbf{i^2}}{\mathbf{i^2}-\mathbf{j^2}}\left(\frac{\pi}{2\mathbf{i}}\right)\cot\left(\frac{\pi}{2\mathbf{i}}\right)-\frac{\mathbf{j^2}}{\mathbf{i^2}-\mathbf{j^2}}\left(\frac{\pi}{2\mathbf{j}}\right)\cot\left(\frac{\pi}{2\mathbf{j}}\right)\right),\end{aligned}$$

where $\mathbf{i} = i/\gcd(i,j)$ *and* $\mathbf{j} = j/\gcd(i,j)$*, and* $\gcd(i,j)$ *denotes the greatest common divisor of* i *and* j*.*

Proof. The proof is in Appendix A. ■

Lemma 1 provided some "probability" interpretations of $p_{\max}(i,j)$ for finite chains. We show that the same interpretation holds for infinite chains.

Lemma 2 $p^{\rightarrow}_{\max}(i,i) = 1$ *and* $p^{\rightarrow}_{\max}(i,j) < 1$ *for* $i \neq j$*.*

Proof. For $i=j$, $\gcd(i,j) = i = j$, so that $\mathbf{i} = \mathbf{j} = 1$ and it remains to show that

$$\frac{4}{\pi^2}\left(2+\sum_{m=2}^{\infty}\frac{4}{(m^2-1)^2}\right) = 1.$$

This can be derived as follows. From the definition of the Riemann ζ function, the following is easily verified:

$$2\sum_{m=2,4,\ldots}^{\infty}\frac{1}{m^s} = 2^{1-s}\zeta(s).$$

Observing that the left-hand side is $2\left(\zeta(s) - \sum_{m=1,3,\ldots} \frac{1}{m^s}\right)$, it follows that

$$\zeta(s)(1-2^{-s}) = \sum_{\mu=1}^{\infty} \frac{1}{(2\mu-1)^s}.$$

Setting $s=2$ and remembering that $\zeta(2) = \pi^2/6$ (Euler formula) give

$$\sum_{\mu=1}^{\infty} \frac{1}{(2\mu-1)^2} = \frac{\pi^2}{8}.$$

Therefore,

$$\sum_{m=2,4,\ldots} \frac{16}{(m^2-1)^2} = 4\left(\frac{\pi^2}{8} + \left(\frac{\pi^2}{8} - 1\right) - 1\right) = \pi^2 - 8.$$

The above and the infinite series representation yields

$$\sqrt{p^{\rightarrow}_{\max}(i,j)} < \frac{4}{\pi^2}\left(2 + \sum_{m=2,4,\ldots} \frac{4}{(m^2-1)^2}\right) = 1.$$

■

It is interesting to observe from the infinite series representation that $p^{\rightarrow}_{\max}(i,j)$ dips when i and j are relatively prime. In particular, relative to the anti-core $j = n+1$, the deepest dips happen at $i=1$ and $i = 2n+1$, since $\gcd(1, n+1) = 1$ and $\gcd(n+1, 2n+1) = 1$. The opposite phenomenon happens when i and j share prime factors. In this case, $\mathbf{i}$ and $\mathbf{j}$ drop, hence by the infinite series representation $p_{\max}(i,j)$ shoots up. This explains the "ripples" in the $\sqrt{p_{\max}(i,j)}$ plots of Fig. 1. Even though this figure is the case of a finite length chain, the "ripple" phenomenon is well explained by the asymptotic formula.

As a word of warning, the "spikes" near the anti-core of Fig. 1 *should not* be misconstrued as "cores." Indeed, the first spike occurs at $j = 87$, so all it is depicting is the trivial fact that $p_{\max}(87,87) = 1$; this implies, by mirror symmetry relative to the middle spin, that $p_{\max}(87,115) = 1$ as well.

Corollary 1 *The diameter of the semi-infinite chain is finite and is achieved along a sequence* $\{i_{k\in\mathbb{N}}\}$ *of prime numbers such that* $\lim_{k\to\infty} i_k = \infty$.

Proof. From the infinite series representation, it is clear that $p^{\rightarrow}_{\max}(i,j) \geq 64/\pi^4$. Hence $\sup_{i\neq j} d^{\rightarrow}(i,j) \leq -\log(64/\pi^4)$. To show that this can be achieved, it suffices to observe that the infinite series goes to 0 along an i-sequence (or j-sequence) of prime numbers. ■

3.2 Doubly-infinite chains

In the doubly infinite chain case, the position of the spins is referenced to ω. Hence, define $i' = i - \omega$ and $j' = j - \omega$. Furthermore, $\mathbf{i}' = i'/\gcd(i',j')$ and $\mathbf{j}' = j'/\gcd(i',j')$.

Theorem 2 *Consider an homogeneous XX chain of odd length $N = 2n+1$ with the positions i', j' of the spins referenced relative to the center $n+1$. Assume i' and j' are positive.*

If both i' and j' are odd or both i' and j' are even with the same power of 2 in their prime number factorization, we have

$$\begin{aligned}\sqrt{p_{\max}^{\leftrightarrow}(i',j')} &= \frac{4}{\pi^2}\left(2+\sum_{m=2,4,\ldots}\frac{4}{(m^2\mathbf{i'}^2-1)(m^2\mathbf{j'}^2-1)}\right)\\ &= \frac{8}{\pi^2}\left(\frac{1}{\mathbf{i'}^2-\mathbf{j'}^2}\left(\mathbf{i'}^2\left(\frac{\pi}{2\mathbf{i'}}\right)\cot\left(\frac{\pi}{2\mathbf{i'}}\right)-\mathbf{j'}^2\left(\frac{\pi}{2\mathbf{j'}}\right)\cot\left(\frac{\pi}{2\mathbf{j'}}\right)\right)\right).\end{aligned}$$

If i' and j' are even with different powers of 2 in their prime number factorization or i' is odd and j' is even,

$$\begin{aligned}\sqrt{p_{\max}^{\leftrightarrow}(i',j')} &= \frac{4}{\pi^2}\left(2+\sum_{m=4,8,\ldots}\frac{4}{(m^2\mathbf{i'}^2-1)(m^2\mathbf{j'}^2-1)}\right)\\ &= \frac{8}{\pi^2}\left(\frac{\mathbf{i'}^2}{\mathbf{i'}^2-\mathbf{j'}^2}\left(\frac{\pi}{4\mathbf{i'}}\right)\cot\left(\frac{\pi}{4\mathbf{i'}}\right)-\frac{\mathbf{j'}^2}{\mathbf{i'}^2-\mathbf{j'}^2}\left(\frac{\pi}{4\mathbf{j'}}\right)\cot\left(\frac{\pi}{4\mathbf{j'}}\right)\right).\end{aligned}$$

Proof. See Appendix B. ■

Theorem 3 *For a homogeneous XX chain of length $N = 2n+1$ with the positions 0, j' of the spins referenced relative to the center $n+1$ and $j' > 0$*

$$\sqrt{p_{\max}^{\leftrightarrow}(0,j')} = \frac{2}{\pi} \approx 0.636619. \tag{4}$$

Proof. The result follows from the integral formulas of Sec. B.3 of Appendix B. ■

As a corollary of this theorem, we show that its asymptotic formula predicts the magnitude of the dip of Figure 1. Observe the following:

$$\begin{aligned}&\sqrt{p_{\max}^{[1:201]}(87,101)}\\ &= \sqrt{p_{\max}^{[1:201]}(101,87)} \quad \text{(by symmetry of the } p_{\max} \text{ function)}\\ &= \sqrt{p_{\max}^{[1:201]}(101,115)} \quad \text{(by mirror symmetry of chain relative to center)}\\ &\approx 0.63 \quad \text{(by inspection of Fig. 1).}\end{aligned}$$

Next, translating the finite chain to the doubly-infinite model, one would expect

$$\sqrt{p_{\max}^{[1:201]}(101,115)} \approx \sqrt{p_{\max}^{\leftrightarrow}(0,14)},$$

which given the above numerical observations holds remarkably accurately. Although $N < \infty$, the dip value of $\sqrt{p_{\max}^{[1:101]}(87,101)}$ is consistent with the asymptotic value given by Theorem 3.

Observe from Theorems 2 and 3 that the "probability" interpretation of $p_{\max}^{\leftrightarrow}$ holds the same way as it did for the semi-infinite chain. The details are left out.

Corollary 2 *The diameter of the doubly-infinite chain is finite and is achieved for* $d^{\leftrightarrow}(0, j') = -2\log(2/\pi)$*.*

Proof. It is easily seen from the infinite series representations of $\sqrt{p^{\leftrightarrow}_{\max}(i', j')}$ in both cases of Theorem 2 that $\sqrt{p^{\leftrightarrow}_{\max}(i'j')} \geq 8/\pi^2$, $\forall i', j' \neq 0$. This together with Theorem 3 implies that the diameter is finite. Furthermore, observe that the bound $8/\pi^2$ is reached along an infinite sequence $\{i'_{k\in\mathbb{N}}\}$ of prime numbers such that $\lim_{k\to\infty} i'_k = \infty$, which guarantees that $\mathbf{i'}_k := i'_k/\gcd(i'_k, j') \to \infty$ at infinity. This together with $2/\pi < 8/\pi^2$ implies that the diameter is $-2\log(2/\pi)$. ■

The fact that the diameter is achieved for one spin at $i' = 0$ reveals the "anti-core."

4 Anti-core

4.1 Minimum probability

Inspired from congestion phenomena in classical communications [8], it was numerically observed in [7] that for chains of odd length $N = 2n+1$ the inertia of the quantum network relative to the spin j, $I^{(\alpha)}(j) := \sum_{i=1}^{N} d^{\alpha}(i, j)$, $\alpha = 2$, is maximal for $j = \omega := n+1$. We now show that a stronger result holds:

$$\arg\max_j d(i, j) = \omega, \quad \forall i \neq \omega,$$

In other words, for each spin other than the center, the center is the farthest away, which of course implies that $I^{(\alpha)}(j)$ is maximum for $j = \omega$. The preceding can be rephrased as

$$\arg\min_j p_{\max}(i, j) = \omega, \quad \forall i \neq \omega.$$

Given the explicit expression for $p_{\max}(i, j)$ in (2), the claim that $\sqrt{p_{\max}(i, j)}$ is achieved for $j = n+1$ amounts to proving the following:

Theorem 4 *For XX chains of odd length* $N = 2n+1$*, we have*

$$\frac{2}{N+1}\sum_{k=1}^{2n+1}\left|\sin\frac{\pi k i}{2(n+1)}\sin\frac{\pi k j}{2(n+1)}\right| \geq \frac{2}{N+1}\sum_{k=1}^{2n+1}\left|\sin\frac{\pi k i}{2(n+1)}\sin\frac{\pi k}{2}\right| \quad (5)$$

as $n \to \infty$*.*

Proof. Firstly, we evaluate the asymptotic value of the right-hand side, that is, the maximum excitation transition probability from spin i to spin $(n+1) = \omega$ (or from spin ω to spin N) for an infinite ($N \to \infty$) chain with XX coupling. From [14, Eq. (16)] or Table 1, we have

$$\lim_{n\to\infty}\sqrt{p_{\max}(i, \omega)} = \lim_{n\to\infty}\frac{1}{n+1}\sum_{k=1}^{2n+1}\left|\sin\frac{\pi k i}{2(n+1)}\sin\frac{\pi k}{2}\right|.$$

The even terms are zero and letting $k = 2l + 1$ we have

$$\sqrt{p_{\max}(i, n+1)} = \frac{1}{n+1} \sum_{l=0}^{n} \left| \sin\left(\frac{\pi i(2l+1)}{2(n+1)}\right) \right|.$$

Setting $x = (2l + 1)/(2(n + 1))$, we have

$$\sqrt{p_{\max}(i, n+1)} = \int_0^1 |\sin(\pi i x)| dx = i \int_0^{1/i} \sin \pi i x dx = \frac{2}{\pi}.$$

Next, from the above and the infinite series representation of Theorem 1, it suffices to show that

$$\frac{4}{\pi^2} \left(2 + \sum_{m \in M} \frac{4}{(m^2 \mathbf{j}^2 - 1)(m^2 \mathbf{i}^2 - 1)} \right) \geq \frac{2}{\pi}.$$

Observe that

$$\frac{4}{\pi^2} \Big(2 + \sum_{m \in M} \frac{4}{(m^2 \mathbf{j}^2 - 1)(m^2 \mathbf{i}^2 - 1)} \Big) \geq \frac{8}{\pi^2} > \frac{2}{\pi}$$

and the Theorem is proved. ■

Thus we have identified spin $\omega = n + 1$ as having minimal probability of any excitation being transferred to or from it. To put it another way, the spin ω is maximally distant from all other spins. We shall call the corresponding probability amplitude "ω-small" and the corresponding distance "ω-large." The "ω-small" property is illustrated in Fig. 1.

4.2 Transport properties

Here we examine the transport properties of the center $\omega = n+1$ and justify its "anti-core" properties. To this end, we consider the path integral representation. Starting with

$$\langle i|e^{-\imath H_1 \tau}|k\rangle = \sum_{\ell=1}^{N} \langle i|e^{-\imath H_1 s}|\ell\rangle\langle \ell|e^{-\imath H_1 (\tau - s)}|k\rangle,$$

we obtain

$$\langle i|e^{-\imath H_1 t}|j\rangle = \sum_{k,\ell=1}^{N} \langle i|e^{-\imath H_1 s}|\ell\rangle\langle \ell|e^{-\imath H_1 (\tau - s)}|k\rangle\langle k|e^{-\imath H_1 (t-\tau)}|j\rangle.$$

By iterating, we get

$$\begin{aligned}\langle i|e^{-\imath H_1 t}|j\rangle &= \sum_{k_1, k_2, \ldots, k_{n-2}=1}^{N} \langle i|e^{-\imath H_1 t_1}|k_1\rangle\langle k_1|e^{-\imath H_1 t_2)}|k_2\rangle \ldots \langle k_{n-2}|e^{-\imath H_1 t_{n-1}}|j\rangle \\ &= \sum_{k_1, k_2, \ldots, k_{n-2}=1}^{N} \prod_{i=1,\ldots,n-1} \langle k_{i-1}|e^{-\imath H_1 t_i}|k_i\rangle\end{aligned}$$

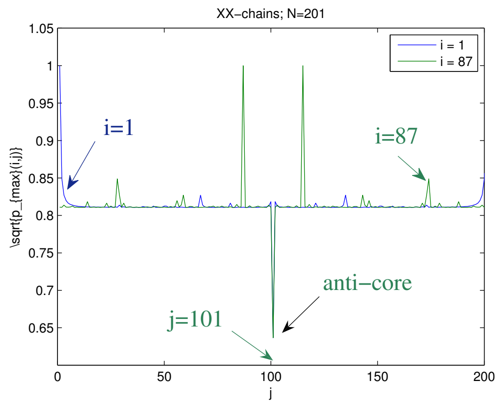

Figure 1: Square root of maximum transition probability between spins $i = 1, 87$ and all j-spins for an XX chain with $N = 201$. The sharp drop at $j = 101$ illustrates the "ω-small" property. The two spikes near the anti-core are *not* congestion cores, as observed in Sec. 3.

with $k_0 = i$, $k_{n-1} = j$, $t_1 + t_2 + \ldots + t_{n-1} = t$, and $n \leq N$. It follows that

$$\begin{aligned}\sqrt{p_t(i,j)} &\leq \sum_{k_1,k_2,\ldots,k_{n-2}=1}^{N} \prod_{i=1,\ldots,n-1} \sqrt{p_{t_i}(k_{i-1},k_i)} \\ &\leq \sum_{k_1,k_2,\ldots,k_{n-2}=1}^{N} \prod_{i=1,\ldots,n-1} \sqrt{p_{\max}(k_{i-1},k_i)}.\end{aligned}$$

Since the above is valid for all t's, we get

$$\sqrt{p_{\max}(i,j)} \leq \sum_{k_1,k_2,\ldots,k_{n-2}=1}^{N} \prod_{i=1,\ldots,n-1} \sqrt{p_{\max}(k_{i-1},k_i)}. \tag{6}$$

The above means that an excitation from the source i to the destination spin j takes all possible length-n paths from i to j, including those paths transiting through $\frac{N+1}{2} = \omega$. For those paths, any term of the form $p_{\max}(\omega, k_i)$ or $p_{\max}(k_{i-1}, \omega)$ is ω-small, making the norm of the product in the right-hand side ω-small. Thus, for any transfer of excitation from i to j, the probability of exciting ω along the way is ω-small. If we consider the probability of excitation of ω as its "congestion," then ω remains clear of congestion, for transfer from any source $i \neq \omega$ to any destination $j \neq \omega$. Thus ω appears to be the anti-thesis of the concept of core; let us agree to call it *"anti-core."*

5 Anti-core in engineered chains

As observed earlier, the diameter of a homogeneous XX chain remains finite even as the length of the chain goes to infinity. We now examine whether we can modify the chain to increase its diameter to infinity. One way to achieve this is to apply a local potential ζ to the central spin ω. This has the effect of perturbing the single excitation Hamiltonian, in turn distorting the original homogeneous distance to d_ζ, so that in the limit $\zeta \to \infty$ the ITC diameter increases *ad infinitum*, hence getting close to the coarse geometry paradigm of dealing with objects of infinite size. The anti-core phenomenon is amplified in the sense that $\lim_{\zeta\to\infty} \sqrt{p_{\max}(1,\omega)} = 0$. This provides a tunneling barrier interpretation of the anti-core.

We prove that the $d_{\zeta\to\infty}$ diameter of the engineered chain goes to ∞ under two different scenarios: $N < \infty$ and $N = \infty$. The $N < \infty$ proof is in the spirit of the main body of the paper; the $N = \infty$ proof is operator-theoretic and relies on the assumption that H_1 is a doubly-infinite matrix, hence eradicating the "border effects."

5.1 Finite Chains

With the applied potential the Hamiltonian in the single excitation subspace becomes

$$H_1^{(\zeta)} = \begin{pmatrix} 0 & 1 & \dots & 0 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 1 & \zeta & 1 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix}. \tag{7}$$

The eigenstructure of this new Hamiltonian yields the new ITC distance d_ζ.

Theorem 5 *For an XX chain of odd length $N < \infty$, $\lim_{\zeta\to\infty} d_\zeta(1,\omega) = \infty$.*

Proof. To emphasize the dependency on the number N of spins, observe that

$$H_1^{(\zeta)} = T_N + \zeta E,$$

where E is the $N \times N$ matrix made up of 0's everywhere except for a 1 in position $\left(\frac{N+1}{2}, \frac{N+1}{2}\right)$; and T_N is the $N \times N$ finite Toeplitz matrix made up of 0's on the diagonal, 1's on the super-diagonal, 1's on the sub-diagonal, and 0's everywhere else. Recall that the determinant of the sum of two matrices equals the sums of the determinants of all matrices made up with some columns of one matrix and the complementary columns of the other matrix. Applying the latter to $\det((\lambda I_N - T_N) - \zeta E))$ yields the characteristic polynomial

$$\det(\lambda I - T_N) - \zeta \left(\det\left(\lambda I - T_{\frac{N-1}{2}}\right)\right)^2.$$

From classical root-locus techniques, it follows that, as $\zeta \to \infty$, *exactly one* eigenvalue λ_N goes to ∞, while the $(N-1)$ remaining ones converge to the roots of $\left(\det\left(\lambda I - T_{\frac{N-1}{2}}\right)\right)^2 = 0$. The eigenvector equations $(T_N + \zeta E)v_k = \lambda_k(\zeta)v_k$ split, asymptotically as $\zeta \to \infty$, into two subsets: one for $\lambda_N \to \infty$ and the others for $\frac{\lambda_k}{\zeta} \to 0$; that is, resp.,

$$Ev_N = \left(\lim_{\zeta\to\infty} \frac{\lambda_N(\zeta)}{\zeta}\right) v_N,$$
$$Ev_k = 0, \quad k \neq N.$$

Next, again from root-locus techniques, it follows that

$$\lim_{\zeta\to\infty} \frac{\lambda_N(\zeta)}{\zeta} = 1,$$

so that $v_{N,k} = 0$, $k \neq \omega$ and $v_{N,\omega} = 1$. On the other hand, it is obvious that $v_{k,\omega} = 0$, $k \neq N$. Therefore

$$p_{\max}(1,\omega) = \sum_{k=1}^{N} |\langle 1|v_k\rangle\langle v_k|\omega\rangle| = 0$$

and $\lim_{\zeta\to\infty} d_\zeta(1,\omega) = \infty$. ■

5.2 Example

To illustrate several important points, we consider a very simple example, which has the advantage of being analytically tractable. Consider the Hamiltonian (7) for the $N = 3$ case. The diagonal matrix of eigenvalues of H_1 can be computed symbolically as

$$\begin{pmatrix} \zeta/2 - (z^2+8)^{1/2}/2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \zeta/2 + (\zeta^2+8)^{1/2}/2 \end{pmatrix}.$$

The normalized eigenvectors are computed as

$$v_1 = \begin{pmatrix} 1/((\zeta/2 - (\zeta^2+8)^{1/2}/2)^2 + 2)^{1/2} \\ (\zeta/2 - (\zeta^2+8)^{1/2}/2)/((\zeta/2 - (\zeta^2+8)^{1/2}/2)^2 + 2)^{1/2} \\ 1/((\zeta/2 - (\zeta^2+8)^{1/2}/2)^2 + 2)^{1/2} \end{pmatrix},$$

$$v_2 = \begin{pmatrix} -2^{1/2}/2 \\ 0 \\ 2^{1/2}/2 \end{pmatrix},$$

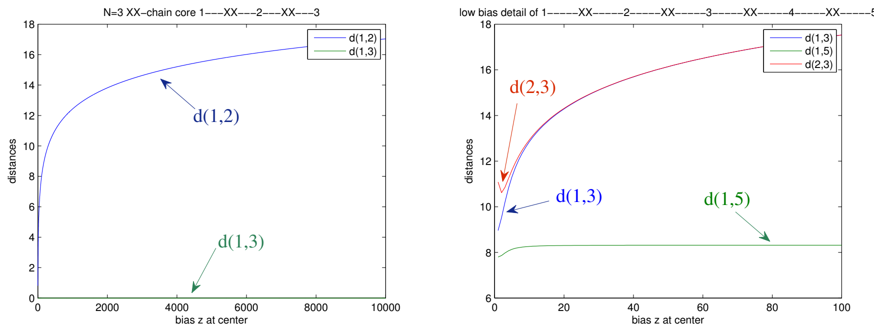

Figure 2: Simple 3-spin (left) and 5-spin (right) chain examples with bias ζ at center showing logarithmic behavior of the distance from the center to the outer spins and vanishing (left) and bounded (right) distance between the outer spins.

$$v_3 = \begin{pmatrix} 1/((\zeta/2 + (\zeta^2+8)^{1/2}/2)^2 + 2)^{1/2} \\ (\zeta/2 + (\zeta^2+8)^{1/2}/2)/((\zeta/2 + (\zeta^2+8)^{1/2}/2)^2 + 2)^{1/2} \\ 1/((\zeta/2 + (\zeta^2+8)^{1/2}/2)^2 + 2)^{1/2} \end{pmatrix}.$$

Using those eigenvectors to symbolically compute $p_{\max}(1,2)$ yields

$$\begin{aligned} & p_{\max}(1,2) = \\ & \Big(\Big| (\zeta/2 - (\zeta^2+8)^{1/2}/2)/((\zeta/2 - (\zeta^2+8)^{1/2}/2)^2 + 2 \Big| \\ + \quad & \Big| (\zeta/2 + (\zeta^2+8)^{1/2}/2)/((\zeta/2 + (\zeta^2+8)^{1/2}/2)^2 + 2 \Big| \Big)^2 \sim 4\zeta. \end{aligned}$$

After symbolic computation of $p_{\max}(1,3)$ and symbolically simplifying the expression, it is observed that $p_{\max}(1,3) = 1$. The results are translated into distances and plotted in Fig. 2, left.

There are several important observations to be made from this simple example:

- The logarithmic behavior of the distance between the anti-core 2 and the outer spin, $d(1,2) = \Theta(\log(\zeta))$, *is confirmed analytically* from the symbolic expression of the eigenvectors. The same applies to $d(1,3) = 0$.

- Because $d(1,3) = 0$ and $d(2,1), d(2,3) \to \infty$ as $\zeta \to \infty$, the geodesic triangle 123 degenerates to the ray $[2,1] = [2,3]$. (A *ray* is an isometric embedding of $[0,\infty)$ to a metric space [3, III.H.3], intuitively meaning that a ray starts at a finite point and extends to infinity along a length minimizing path.) As such, because $\triangle 123$ is "flat," it is a Gromov δ-slim triangle. (A triangle is δ-slim [3, III.H.1] if any edge is contained in the union of the δ-neighborhoods of the other two edges.) Thus the 123 chain is a, albeit trivial, Gromov hyperbolic space. (A metric space is Gromov hyperbolic [3, III.H.1] if there exists a $\delta < \infty$ such that all of its geodesic triangles are δ-slim.)

- The rays $[2,1]$ and $[2,3]$ are going to infinity while keeping their Hausdorff distance finite, in fact vanishing. So they converge to the same point on the Gromov boundary. (The Gromov boundary [3, III.H.3] is the equivalence class of rays keeping their distance finite.) Thus the 123 chain has its Gromov boundary reduced to a singleton.

- The preceding fact (Gromov boundary reduced to a singleton) is the major topological discrepancy between classical and quantum networks. Most classical networks have at least two points in their Gromov boundary, creating a core [2] as opposed to the anti-core of quantum communications.

The preceding 3-spin example has been extended to the same 5-spin case (Fig. 2, right) with all results *proved* by symbolic manipulations, which unfortunately become prohibitively long to be included here. The results are the same, except that the distance between the outer spins remains finite (rather than vanishing), but this suffices to come to the conclusion that the chain has only one point in its Gromov boundary. We conjecture that this is a general feature.

5.3 Infinite Chains

A proof of the infinite diameter property of the engineered chain with bias ζ at the center ω can be developed under infinite number of spins hypothesis, $N \to \infty$. Indeed, in this case, H_1 becomes the doubly infinite Toeplitz (also referred to as Laurent or multiplication) operator T_s with symbol $s(\exp(i\theta)) = \exp(i\theta) + \exp(-i\theta)$, and $H_1^{(\zeta)}$ is a compact perturbation ζE of T_s, where $E = |e\rangle\langle e|$ with $e = (\ldots 0, 0, 1, 0, 0 \ldots)'$ the unit basis vector of the Hilbert space $\ell^2(-\infty, +\infty)$ of square summable doubly infinite sequences. By a well known perturbation theory result, the spectrum of $H_1^{(\zeta)} : \ell^2(-\infty, +\infty) \to \ell^2(-\infty, +\infty)$ consists of the interval $s([0, 2\pi)) = [-2, +2]$ plus another eigenvalue of finite multiplicity that converges asymptotically to ζ. The eigen-equation $H_1^{(\zeta)} v_\lambda = \lambda v_\lambda$ becomes

$$(T_s - \lambda I)v_\lambda = -\zeta E v_\lambda = -\zeta v_{\lambda,\omega} e,$$

where $v_{\lambda,\omega}$ denotes the central component of the eigenvector v_λ. In the Fourier or z-domain, $T_s - \lambda I$ is just the multiplication by $(z + z^{-1} - \lambda)$ operator. Therefore, the above can be resolved as

$$\hat{v}_\lambda = \frac{-\zeta v_{\lambda,\omega}}{z + z^{-1} - \lambda},$$

where $\hat{v}_\lambda$ denotes the Fourier or z-transform of v_λ. Taking $\lambda \in (-2, 2)$, it is easily verified that the Laurent expansion of the above converges on the unit circle; hence the inverse Fourier or z-transform is in $\ell^2(-\infty, +\infty)$. This provides an example of the rather unusual circumstance under which a *continuous* spectrum (here $[-2, +2]$ of T_s) is converted in to *pure point* spectrum (here $(-2, +2)$ of $T_s + \zeta E$) by a compact perturbation.

The formula for the probability becomes

$$p_{\max}(i,j) = \int_{-2}^{+2} |\langle v_\lambda|i\rangle\langle j|v_\lambda\rangle| d\lambda + |\langle v_\zeta|i\rangle\langle j|v_\zeta\rangle|,$$

where v_ζ is the eigenvector corresponding to the asymptotic eigenvalue ζ. Here, we are specifically interested in the case $p_{\max}(\omega,\infty)$ of the probability of transition from the center to infinity. Take $\lambda \in (-2,+2)$. We need to evaluate $\langle v_\lambda|\omega\rangle$ and $\langle v_\lambda|\infty\rangle$. Recall that Parseval's theorem $\sum_{m=-\infty}^{+\infty} a_m b_m = \frac{1}{2\pi i}\oint \hat{a}(z)\hat{b}(z^{-1})\frac{dz}{z}$ allows us to compute an inner product by residue calculation. Using the recipe yields

$$\begin{aligned}\langle v_\lambda|\omega\rangle &= \frac{1}{2\pi\imath}\oint 1 \frac{-\zeta v_{\lambda,\omega}}{z+z^{-1}-\lambda}\frac{dz}{z} = \frac{1}{2\pi\imath}\oint 1 \frac{-\zeta v_{\lambda,\omega}}{z^2-\lambda z+1} dz \\ &= \text{Residue}\left(\frac{-\zeta v_{\lambda,\omega}}{z^2-\lambda z+1}\right)_{p,\bar{p}},\end{aligned}$$

where $p,\bar{p}$, with $|p|<1, |\bar{p}|<1$, are the poles of the integrand, that is, the zeros of $z^2-\lambda z+1$. This yields

$$\langle v_\lambda|\omega\rangle = \frac{-\zeta v_{\lambda,\omega}}{p-\bar{p}} + \frac{-\zeta v_{\lambda,\omega}}{\bar{p}-p} = 0.$$

Next, we look at the term $\langle v_\lambda|\infty\rangle$ as the limit of $\langle v_\lambda|M\rangle$ as $M\to\infty$. We have

$$\begin{aligned}\langle v_\lambda|M\rangle &= \frac{1}{2\pi\imath}\oint \frac{-\zeta v_{\lambda,\omega}}{z+z^{-1}-\lambda} z^M \frac{dz}{z} = \text{Residue}\left(\frac{-\zeta v_{\lambda,\omega} z^M}{z^2-\lambda z+1}\right)_{p,\bar{p}} \\ &= \frac{-\zeta v_{\lambda,\omega} p^M}{p-\bar{p}} + \frac{-\zeta v_{\lambda,\omega} \bar{p}^M}{\bar{p}-p}.\end{aligned}$$

Since $|p|<1$, the limit of the above as $M\to\infty$ vanishes. Last, we look at the isolated eigenvalue case, $|\langle v_k|\omega\rangle\langle M|v_k\rangle|$. Since $v_k \approx e$, and the excited state $|M\rangle$ is a basis vector orthogonal to e, we have $\langle M|v_k\rangle = 0$. Hence the probability $p_{\max}(\infty,\omega) = 0$ and the distance $d_\zeta(\omega,\infty)$ is infinity.

6 Discussion and Conclusions

The early numerical observation [7] that homogeneous odd length N-spin chains have an "anti-gravity" center has been *analytically* confirmed in the $N\to\infty$ limit by developing closed-form formulas for the asymptotic maximum excitation transfer probability, and by showing that the anti-core has the lowest probability of being excited or of transmitting its excitation. As shown in Sec. 3, the phenomena exhibited in Fig. 1 can be accurately explained by the $N=\infty$ asymptotic formula.

The existence of an anti-core at the center of a linear array of spins shows that excitations in a spin network do not propagate as they would in a classical network. In a classical linear network any excitation in one half of the chain must transit through the center to reach the other half, and the center would thus be expected to be a congestion core. In quantum networks, however, excitations can be transferred from one end of a chain to the other without passing through the center due to the intrinsic entanglement present in the eigenstates of the system. When a single excitation is created in one location what is really created is a wavepacket, which is a superposition of many eigenstates of the system Hamiltonian that subsequently evolve and interfere. High probability of transmission requires constructive interference at any particular node at some time, and the existence of an anti-core shows that, surprisingly, there is least constructive interference for the center of the chain.

As we have also shown, it is possible to engineer chains such that the diameter of the chain goes to infinity even if the physical number of spins is finite. The simplest way to achieve this is by applying a bias to the central spin in an odd-length chain. By increasing the bias we can increase the diameter even for a finite chain and achieve infinite diameter in the limit of infinite bias. This can be explained in terms of the bias moving the central spin further and further away from the other spins and therefore effectively decoupling the chains. However, for any finite bias, no matter how large, an excitation in one half of the chain can tunnel through the obstruction in the center given sufficient time, allowing almost perfect excitation transfer between the end spins of the engineered chain.

Such finite length, infinite diameter chains lend themselves to a coarse Gromov analysis, as Section 5 shows. The specific feature, demonstrated on chains of limited length but conjectured to hold for longer chains, is a Gromov boundary reduced to a singleton. This strongly contrasts with the classical network paradigm of a Gromov boundary with at least two points, creating the congestion core [2]. Although there is early indication that the difference in cardinalities of the Gromov boundaries might be at least part of the explanation of the core versus anti-core discrepancy, more analysis is needed to prove a general fact and is left for further research.

A Proof of Theorem 1 (semi-infinite chain)

We proceed from

$$\sqrt{p_{\max}^{[1:N]}(i,j)} = \frac{2}{N+1} \sum_{k=1}^{2n+1} \left| \sin \frac{\pi k i}{2(n+1)} \sin \frac{\pi k j}{2(n+1)} \right|, \tag{8}$$

where $N = 2n+1$ is the (odd) number of spins and i and j are the positions of the two spins *relative to the left-most spin (1).* Since the number of spins will be taken to infinity, we make the dependency on such number explicit.

A.1 Asymptotic maximum transfer probability

Defining $x'_k = k/(2(n+1))$ for $k = 0, \ldots, 2n+1$, the right-hand side of (8) becomes

$$\sqrt{p_{\max}^{[1:N]}(i,j)} = 2 \sum_{k=1}^{2n+1} |\sin \pi x'_k i| \, |\sin \pi x'_k j| \, (x'_k - x'_{k-1}).$$

Taking the limit $n \to \infty$, the above becomes

$$\begin{aligned}\sqrt{p_{\max}^{\rightarrow}(i,j)} &:= \lim_{n\to\infty} \sqrt{p_{\max}^{[1:N]}(i,j)} \\ &= 2\int_0^1 |\sin \pi i x'||\sin \pi j x'| \, dx' = 4\int_0^{1/2} |\sin 2\pi i x||\sin 2\pi j x| \, dx.\end{aligned}$$

Since $|\sin 2\pi i x| = \left|\sin\left(2\pi i\left(x+\frac{1}{2}\right)\right)\right|$, the above becomes

$$\begin{aligned}\sqrt{p_{\max}^{\rightarrow}(i,j)} =& 2\int_0^{1/2} |\sin 2\pi i x||\sin 2\pi j x| dx \\ & + 2\int_0^{1/2} \left|\sin 2\pi i\left(\tfrac{1}{2}+x\right)\right| \left|\sin 2\pi j\left(\tfrac{1}{2}+x\right)\right| dx \\ =& 2\int_0^1 |\sin 2\pi i x||\sin 2\pi j x| dx.\end{aligned}$$

Next, observe that $|\sin 2\pi i x| = \sin(2\pi i x)s_i(x)$ where $s_i(x)$ is a periodic square wave with fundamental $\sin 2\pi i x$ and Fourier decomposition

$$s_i(x) = \frac{4}{\pi} \sum_{p=1,3,\ldots} \frac{1}{p} \sin 2\pi i p x.$$

Therefore, the absolute values in the integral representation of $\sqrt{p_{\max}(i,j)}$ can be removed as follows:

$$\sqrt{p_{\max}^{\rightarrow}(i,j)} = \frac{32}{\pi^2} \sum_{p,q=1,3,\ldots} \frac{1}{pq} \int_0^1 (\sin 2\pi i x \sin 2\pi i p x)(\sin 2\pi j x \sin 2\pi j q x) dx.$$

Next, utilizing several well-known trigonometric identities, we get, successively,

$$
\begin{aligned}
&\sqrt{p^{\rightarrow}_{\max}(i,j)}\\
=&\frac{8}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_0^1(\cos 2\pi i(p-1)x-\cos 2\pi i(p+1)x)\\
&\qquad\qquad\qquad\cdot(\cos 2\pi j(q-1)x-\cos 2\pi j(q+1)x)\,dx\\
=&\frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_0^1((\cos 2\pi(i(p-1)-j(q-1))x+\cos 2\pi(i(p-1)+j(q-1))x)\\
&\qquad-(\cos 2\pi(i(p-1)-j(q+1)x)+\cos 2\pi(i(p-1)+j(q+1))x)\\
&\qquad-(\cos 2\pi(i(p+1)-j(q-1))x+\cos 2\pi(i(p+1)+j(q-1))x)\\
&\qquad+(\cos 2\pi(i(p+1)-j(q+1))x+\cos 2\pi(i(p+1)+j(q+1))x)\,)dx\\
=&\frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}(\mathbb{1}_{i(p-1)-j(q-1)=0}+\mathbb{1}_{i(p-1)+j(q-1)=0}\\
&\qquad-\mathbb{1}_{i(p-1)-j(q+1)=0}-\mathbb{1}_{i(p-1)+j(q+1)=0}\\
&\qquad-\mathbb{1}_{i(p+1)-j(q-1)=0}-\mathbb{1}_{i(p+1)+j(q-1)=0}\\
&\qquad+\mathbb{1}_{i(p+1)-j(q+1)=0}+\mathbb{1}_{i(p+1)+j(q+1)=0}\,),
\end{aligned}
$$

where $\mathbb{1}_L$ takes the value 1 if the logical statement L is true and 0 otherwise.

Observe that, since $i,p,j,q\geq 1$,

$$\mathbb{1}_{i(p-1)+j(q+1)=0}=0,\ \mathbb{1}_{i(p+1)+j(q-1)=0}=0,\ \mathbb{1}_{i(p+1)+j(q+1)=0}=0$$

and that $\mathbb{1}_{i(p-1)+j(q-1)=0}$ takes the value 1 only for $p=q=1$. Thus, in the above, the sum over p,q of the right-hand side terms amounts to 1.

Next, we look at the left-hand side terms of the sum over p,q. For such a statement as $i(p-1)-j(q-1)=0$ to be true, we need $p-1=m\mathbf{j}$ and $q-1=m\mathbf{i}$ for some $m\in\mathbb{N}$, where $\mathbf{j}=j/\gcd(i,j)$ and $\mathbf{i}=i/\gcd(i,j)$. This yields $p=m\mathbf{j}+1$ and $q=m\mathbf{i}+1$. Observe that $m=0$ is an admissible value, since this yields $p=1$, $q=1$ and hence $i(p-1)-j(q-1)=0$. Recapitulating and following up with the same argument on the other logical statements, we find

$$
\begin{aligned}
i(p-1)-j(q-1)=0 &\Leftrightarrow \begin{cases} p=m\mathbf{j}+1,\\ q=m\mathbf{i}+1,\end{cases}\\
i(p-1)-j(q+1)=0 &\Leftrightarrow \begin{cases} p=m\mathbf{j}+1,\\ q=m\mathbf{i}-1,\end{cases}\\
i(p+1)-j(q-1)=0 &\Leftrightarrow \begin{cases} p=m\mathbf{j}-1,\\ q=m\mathbf{i}+1,\end{cases}\\
i(p+1)-j(q+1)=0 &\Leftrightarrow \begin{cases} p=m\mathbf{j}-1,\\ q=m\mathbf{i}-1.\end{cases}
\end{aligned}
$$

Note that, since $p,q\geq 1$, the solution $m=0$ is not admissible for the second, third, and forth cases, since this would entail either p or q or both of them to equal -1. In addition, p and q must be restricted to be odd, that is, both $m\mathbf{i}$ and $m\mathbf{j}$ must be even. Since $\mathbf{i}$ and $\mathbf{j}$ are relatively prime, they cannot be both even; thus m must be even. The solution $m = 0$ is still acceptable for the first case, since it makes both p and q odd.

To summarize, the sum over $p, q = 1, 3, \ldots$ reduces to 2 plus a sum over $m \in \mathbb{N}^*$, subject to the restrictions that $m\mathbf{i} - 1 \neq 0$ and $m\mathbf{j} - 1 \neq 0$. Changing the sum over p, q to a sum over m, it follows that

$$\begin{aligned}\sqrt{p^{\rightarrow}_{\max}(i,j)} =& \frac{4}{\pi^2}\left[2 + \sum_{m\in M} \frac{1}{(m\mathbf{j}+1)(m\mathbf{i}+1)} - \frac{1}{(m\mathbf{j}+1)(m\mathbf{i}-1)}\right.\\ &\left. - \frac{1}{(m\mathbf{j}-1)(m\mathbf{i}+1)} + \frac{1}{(m\mathbf{j}-1)(m\mathbf{i}-1))}\right]\\ =& \frac{4}{\pi^2}\left(2 + \sum_{m\in M} \frac{4}{(m^2\mathbf{j}^2-1)(m^2\mathbf{i}^2-1)}\right), \end{aligned} \tag{9}$$

where $M = \{m \in \mathbb{N}^* : m \text{ is even}, m^2\mathbf{i}^2 - 1 \neq 0, m^2\mathbf{j}^2 - 1 \neq 0\}$. This proves the infinite series representation of Theorem 1. ■

A.2 Closed form of asymptotic transfer probability

Next, we express the infinite series of Theorem 1 in terms of elementary functions. First, consider the partial fraction decomposition

$$\frac{1}{(m^2\mathbf{j}^2-1)(m^2\mathbf{i}^2-1)} = \frac{A(\mathbf{i},\mathbf{j})}{(m^2\mathbf{j}^2-1)} + \frac{A(\mathbf{j},\mathbf{i})}{(m^2\mathbf{i}^2-1)}, \qquad A(\mathbf{i},\mathbf{j}) := \frac{\mathbf{i^2}}{\mathbf{j^2}-\mathbf{i^2}}.$$

Next, observe the following lemma:

Lemma 3

$$\sum_{m=2,4,6,\ldots} \frac{1}{(m^2\mathbf{i}^2-1)} = \frac{1}{2}\left(1 - \frac{\pi}{2\mathbf{i}}\cot\frac{\pi}{2\mathbf{i}}\right).$$

Proof. In the known expression for the cotangent,

$$\pi\cot(\pi z) = \frac{1}{z} + 2z\sum_{n=1}^{\infty} \frac{1}{z^2-n^2},$$

set $z = 1/2\mathbf{i}$. This yields

$$\sum_{n=1}^{\infty} \frac{1}{(2n\mathbf{i})^{\mathbf{2}} - \mathbf{1}} = \frac{1}{2}\left(1 - \left(\frac{\pi}{2\mathbf{i}}\right)\cot\left(\frac{\pi}{2\mathbf{i}}\right)\right).$$

Setting $m = 2n$ yields the result. ■

Putting everything together using the lemma yields

$$\sqrt{p^{\rightarrow}_{\max}(i,j)} = \frac{8}{\pi^2}\left(\frac{\mathbf{i^2}}{\mathbf{i^2}-\mathbf{j^2}}\left(\frac{\pi}{2\mathbf{i}}\right)\cot\left(\frac{\pi}{2\mathbf{i}}\right) - \frac{\mathbf{j^2}}{\mathbf{i^2}-\mathbf{j^2}}\left(\frac{\pi}{2\mathbf{j}}\right)\cot\left(\frac{\pi}{2\mathbf{j}}\right)\right)$$

and Theorem 1 is proved. ■

B Proofs of Theorem 2 (doubly-infinite chain)

We proceed from

$$\sqrt{p_{\max}^{[1:N]}(i,j)} = \frac{2}{N+1}\sum_{k=1}^{2n+1}\left|\sin\frac{\pi k i}{2(n+1)}\sin\frac{\pi k j}{2(n+1)}\right|,$$

where $N = 2n+1$ is the (odd) number of spins and i and j are the positions of the two spins *relative to the central spin (n+1)*. Since the number of spins will be taken to infinity, we make the dependency on such number explicit.

B.1 Referencing max. transfer probability to anti-core

The first operation is to do the change of variable $k' = k-(n+1)$ and convert the sum as k goes from 1 to $2n+1$ to a sum where k' goes from $-n$ to $+n$. After some manipulation, the following is found:

$$\sqrt{p_{\max}^{[1:N]}(i,j)} = \frac{2}{N+1}\sum_{k'=-n}^{+n}\left|f\left(\frac{\pi k' i}{2(n+1)}\right)g\left(\tfrac{\pi k' j}{2(n+1)}\right)\right|,$$

where f, g are given in Table 2.

Table 2: The functions f and g.

	$f(\cdot)$	$g(\cdot)$
i,j even	$\sin(\cdot)$	$\sin(\cdot)$
i,j odd	$\cos(\cdot)$	$\cos(\cdot)$
i even, j odd	$\sin(\cdot)$	$\cos(\cdot)$
i odd, j even	$\cos(\cdot)$	$\sin(\cdot)$

The next step is the change of variables $i' = i-(n+1)$ and $j' = j-(n+1)$. With this change of variables, the position of the spins are relative to the anti-core, $n+1$. This change of variables leads to the following:

$$\begin{aligned}\sqrt{p_{\max}^{[-n:+n]}(i',j')} &:= \sqrt{p_{\max}^{[1:N]}(i'+(n+1),j'+(n+1))}\\ &= \frac{2}{N+1}\sum_{k'=-n,\text{even}}^{+n}\left|f\left(\frac{\pi k' i'}{2(n+1)}\right)g\left(\frac{\pi k' j'}{2(n+1)}\right)\right|\\ &\quad+\frac{2}{N+1}\sum_{k'=-n,\text{odd}}^{+n}\left|\bar{f}\left(\frac{\pi k' i'}{2(n+1)}\right)\bar{g}\left(\frac{\pi k' j'}{2(n+1)}\right)\right|,\end{aligned}$$

where f, g are still given by Table 2 and $\bar{f}(\cdot) = \cos(\cdot), \sin(\cdot)$ whenever $f(\cdot) = \sin(\cdot), \cos(\cdot)$, resp., with the same definition for $\bar{g}$. Since the most recent formula is in terms of i', j', we rewrite Table 2 in terms of i', j' and n in Table 3.

Table 3: The functions f and g in terms of i', j' and n.

	$f(\cdot)$	$g(\cdot)$
$i'+n, j'+n$ odd	$\sin(\cdot)$	$\sin(\cdot)$
$i'+n, j'+n$ even	$\cos(\cdot)$	$\cos(\cdot)$
$i'+n$ odd, $j'+n$ even	$\sin(\cdot)$	$\cos(\cdot)$
$i'+n$ even, $j'+n$ odd	$\cos(\cdot)$	$\sin(\cdot)$

B.2 Towards asymptotic maximum probability

In anticipation of letting $n \to \infty$, define $x_{k'} := \frac{k'}{4(n+1)}$ and the preceding sums can be rewritten as

$$\sqrt{p_{\max}^{[-n:+n]}(i',j')} = 2 \sum_{k'=-n,\text{even}}^{+n} \left| f\left(2\pi x_{k'} i'\right) g\left(2\pi x_{k'} j'\right)\right| \left(x_{k'+2} - x_{k'}\right)$$
$$+ 2 \sum_{k'=-n,\text{odd}}^{+n} \left| \bar{f}\left(2\pi x_{k'} i'\right) \bar{g}\left(2\pi x_{k'} j'\right)\right| \left(x_{k'+2} - x_{k'}\right).$$

Letting $n \to \infty$ yields

$$\sqrt{p_{\max}^{\leftrightarrow}(i',j')} := \lim_{n\to\infty} \sqrt{p_{\max}^{[-n:+n]}(i',j')}$$
$$= 2\int_{-1/4}^{+1/4} |f(2\pi x i')g(2\pi x j')|dx + 2\int_{-1/4}^{+1/4} |\bar{f}(2\pi x i')\bar{g}(2\pi x j')|dx.$$

In order to make the integrations more straightforward and to follow a procedure that parallels the one of Appendix A, it is convenient to change the integration limits by making use of the periodicity of the integrands as functions of x. Observe that both fg and $\bar{f}\bar{g}$ have decompositions in terms of sines or cosines of arguments $2\pi x(i' \pm j')$. Write the generic term as $\left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} (2\pi x(i' \pm j'))$. If $i' \pm j'$ is even, observe that $\left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} (2\pi(x+1/2)(i' \pm j')) = \left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} (2\pi x(i' \pm j'))$. If $i' \pm j'$ is odd, $\left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} (2\pi(x+1/2)(i' \pm j')) = -\left\{ \begin{array}{c} \sin \\ \cos \end{array} \right\} (2\pi x(i' \pm j'))$. In either case, $|fg|$ and $|\bar{f}\bar{g}|$ have period $1/2$. With this property, the previous integrals can be rewritten as

$$\sqrt{p_{\max}^{\leftrightarrow}(i',j')} = \int_{-1/2}^{+1/2} |f(2\pi x i')g(2\pi x j')|dx + \int_{-1/2}^{+1/2} |\bar{f}(2\pi x i')\bar{g}(2\pi x j')|dx. \tag{10}$$

Observe that $p_{\max}(i',j') \leq 1$, as easily seen from a Cauchy-Schwarz argument. Also observe that $p_{\max}(i',i') = 1$; indeed, if $i' = j'$, Table 3 reveals that the integrands are of the form $|\cos(2\pi i'x)\cos(2\pi i'x)|$ or $|\sin(2\pi i'x)\sin(2\pi i'x)|$, from which the assertion is trivial.

The next step is to make $|f|$, $|g|$, $|\bar{f}|$, $|\bar{g}|$ more manageable by expressing them as $f(2\pi x i')s_{i'}(x)$, $g(2\pi x j')s_{j'}(x)$, $\bar{f}(2\pi x i')s_{i'}(x)$, $\bar{g}(2\pi x j')s_{j'}(x)$ if f, g, $\bar{f}$, $\bar{g}$ are sines and by $f(2\pi x i')c_{i'}(x)$, $g(2\pi x j')c_{j'}(x)$, $\bar{f}(2\pi x i')c_{i'}(x)$, $\bar{g}(2\pi x j')c_{j'}(x)$ if they are cosines. In the preceding, $s_{i'}(x)$ and $c_{i'}(x)$ are odd and even, resp., square waves of unit amplitude and of period 1, with Fourier decompositions

$$s_{i'}(x) = \frac{4}{\pi} \sum_{p=1,3,\ldots} \frac{1}{p} \sin(2\pi i' p x),$$

$$c_{i'}(x) = \frac{4}{\pi} \sum_{p=1,3,\ldots} \frac{(-1)^{\frac{p-1}{2}}}{p} \cos(2\pi i' p x).$$

At this stage, it is necessary to be more specific as to what f, g, $\bar{f}$, $\bar{g}$ are.

B.3 Consistency of asymptotic max. transfer probability

B.3.1 i' and j' even

If i' and j' are even, and if we let $n \to \infty$ along the even number subsequence of $\mathbb{N}$, we need to take $f(\cdot) = \cos(\cdot)$ and $g(\cdot) = \cos(\cdot)$, as seen from Table 3, together with $\bar{f}(\cdot) = \sin(\cdot)$ and $\bar{g}(\cdot) = \sin(\cdot)$. If on the other hand, we let $n \to \infty$ along the odd number subsequence of $\mathbb{N}$, we need to take $f(\cdot) = \sin(\cdot)$ and $g = \sin(\cdot)$, together with $\bar{f}(\cdot) = \cos(\cdot)$ and $\bar{g}(\cdot) = \cos(\cdot)$. However, because of the symmetry of formula (10), both subsequences yield the same result:

$$\begin{aligned}
&\sqrt{p^{\leftrightarrow}_{\max}(i', j')} \\
&= \int_{-1/2}^{+1/2} |\cos(2\pi x i')\cos(2\pi x j')| dx + \int_{-1/2}^{+1/2} |\sin(2\pi x i')\sin(2\pi x j')| dx \\
&= \int_{-1/2}^{+1/2} \cos(2\pi x i')c_{i'}(x)\cos(2\pi x j')c_{j'}(x) dx \\
&\qquad\qquad + \int_{-1/2}^{+1/2} \sin(2\pi x i')s_{i'}(x)\sin(2\pi x j')s_{j'}(x) dx.
\end{aligned}$$

B.3.2 i' and j' odd

The argument is the same as before and the preceding formula still holds.

B.3.3 i' odd and j' even

From Table 3, we could let $n \to \infty$ along the even number subsequence of $\mathbb{N}$, in which case we need to take $f(\cdot) = \sin(\cdot)$ and $g(\cdot) = \cos(\cdot)$. If we let $n \to \infty$ along the odd number subsequence of $\mathbb{N}$, we need to take $f(\cdot) = \cos(\cdot)$ and

$g(\cdot) = \sin(\cdot)$. In either case, because of the symmetry of (10), the result is the same and is given by

$$\begin{aligned}
&\sqrt{p_{\max}^{\leftrightarrow}(i', j')} \\
&= \int_{-1/2}^{+1/2} |\sin(2\pi x i')\cos(2\pi x j')| dx + \int_{-1/2}^{+1/2} |\cos(2\pi x i')\sin(2\pi x j')| dx \\
&= \int_{-1/2}^{+1/2} \sin(2\pi x i') s_{i'}(x) \cos(2\pi x j') c_{j'}(x) dx \\
&\qquad\qquad + \int_{-1/2}^{+1/2} \cos(2\pi x i') c_{i'}(x) \sin(2\pi x j') s_{j'}(x) dx.
\end{aligned}$$

B.3.4 i' even and j' odd

The formula of the preceding section remains valid. To prove it, just interchange the role of i' and j'.

B.4 Towards integration by quadrature

From the above, it follows that all cases share a few quadrature integrals:

$$\begin{aligned}
&\int_{-1/2}^{+1/2} \sin(2\pi x i') s_{i'}(x) \sin(2\pi x j') s_{j'}(x) dx \\
&= \frac{16}{\pi^2} \sum_{p,q=1,3,\ldots} \frac{1}{pq} \int_{-1/2}^{1/2} \sin(2\pi i' x) \sin(2\pi i' p x) \sin(2\pi j' x) \sin(2\pi j' q x) dx \\
&= \frac{4}{\pi^2} \sum_{p,q} \frac{1}{pq} \int_{-1/2}^{1/2} (\cos(2\pi i'(p-1)x) - \cos(2\pi i'(p+1)x)) \\
&\qquad\qquad \cdot (\cos(2\pi j'(q-1)x) - \cos(2\pi j'(q+1)x)) dx \\
&= \frac{2}{\pi^2} \sum_{p,q} \frac{1}{pq} \int_{-1/2}^{1/2} (\sum \cos(2\pi(i'(p-1) \pm j'(q-1))x) \\
&\qquad\qquad - \sum \cos(2\pi(i'(p-1) \pm j'(q+1))x) \\
&\quad - \sum \cos(2\pi(i'(p+1) \pm j'(q-1))x) + \sum \cos(2\pi(i'(p+1) \pm j'(q+1))x)) dx.
\end{aligned}$$

The right-hand side of the last equality involves expressions like $\cos(2\pi(a + b)x) + \cos(2\pi(a - b)x)$. To simplify the notation, we wrote such expressions as $\sum \cos(2\pi(a \pm b)x)$.

$$(-1)^{\frac{p+q}{2}-1}\int_{-1/2}^{+1/2}\cos(2\pi xi')c_{i'}(x)\cos(2\pi xj')c_{j'}(x)dx$$

$$= \frac{16}{\pi^2}\sum_{p,q=1,3,\ldots}\frac{1}{pq}\int_{-1/2}^{1/2}\cos(2\pi i'x)\cos(2\pi i'px)\cos(2\pi j'x)\cos(2\pi j'qx)dx$$

$$= \frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_{-1/2}^{1/2}(\cos(2\pi i'(p+1)x)+\cos(2\pi i'(p-1)x))$$

$$\cdot(\cos(2\pi j'(q+1)x)+\cos(2\pi j'(q-1)x))dx$$

$$= \frac{2}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_{-1/2}^{1/2}(\sum\cos(2\pi(i'(p+1)\pm j'(q+1))x)$$

$$+\sum\cos(2\pi(i'(p+1)\pm j'(q-1))x)$$

$$+\sum\cos(2\pi(i'(p-1)\pm j'(q+1))x)+\sum\cos(2\pi(i'(p-1)\pm j'(q-1))x))dx;$$

$$(-1)^{\frac{q-1}{2}}\int_{-1/2}^{+1/2}\sin(2\pi xi')s_{i'}(x)\cos(2\pi xj')c_{j'}(x)dx$$

$$= \frac{16}{\pi^2}\sum_{p,q=1,3,\ldots}\frac{1}{pq}\int_{-1/2}^{1/2}\sin(2\pi i'x)\sin(2\pi i'px)\cos(2\pi j'x)\cos(2\pi j'qx)dx$$

$$= \frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_{-1/2}^{1/2}(\cos(2\pi i'(p-1)x)-\cos(2\pi i'(p+1)x))$$

$$\cdot(\cos(2\pi j'(q-1)x)+\cos(2\pi j'(q+1)x))dx$$

$$= \frac{2}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_{-1/2}^{1/2}(\sum\cos(2\pi(i'(p-1)\pm j'(q-1))x)$$

$$+\sum\cos(2\pi(i'(p-1)\pm j'(q+1))x)$$

$$-\sum\cos(2\pi(i'(p+1)\pm j'(q-1))x)-\sum\cos(2\pi(i'(p+1)\pm j'(q+1))x))dx;$$

$$
\begin{aligned}
&(-1)^{\frac{p-1}{2}} \int_{-1/2}^{+1/2} \cos(2\pi x i') c_{i'}(x) \sin(2\pi x j') s_{j'}(x) dx \\
&= \frac{16}{\pi^2} \sum_{p,q=1,3,\dots} \frac{1}{pq} \int_{-1/2}^{1/2} \cos(2\pi i' x) \cos(2\pi i' p x) \sin(2\pi j' x) \sin(2\pi j' q x) dx \\
&= \frac{4}{\pi^2} \sum_{p,q} \frac{1}{pq} \int_{-1/2}^{1/2} (\cos(2\pi i'(p+1)x) + \cos(2\pi i'(p-1)x)) \\
&\qquad \cdot (\cos(2\pi j'(q-1)x) - \cos(2\pi j'(q+1)x)) dx \\
&= \frac{2}{\pi^2} \sum_{p,q} \frac{1}{pq} \int_{-1/2}^{1/2} (\sum \cos(2\pi(i'(p+1) \pm j'(q-1))x) \\
&\qquad - \sum \cos(2\pi(i'(p+1) \pm j'(q+1))x) \\
&\quad + \sum \cos(2\pi(i'(p-1) \pm j'(q-1))x) - \sum \cos(2\pi(i'(p-1) \pm j'(q+1))x)) dx.
\end{aligned}
$$

B.5 Asymptotic max. transfer probability around anti-core

Here we proceed from the general formula (10) for $\sqrt{p_{\max}^{\leftrightarrow}(i',j')}$, utilize the quadrature integrals of the preceding section, and derive, first, an infinite series representation of the asymptotic maximum transfer probability and, finally, a representation in terms of special functions. Since the general formula (10) is in terms of function f, g, $\bar{f}$, $\bar{g}$ that depend on whether i' and j' are even or odd (see Section B.3), it is necessary to examine each case in particular. From Section B.3, it follows that the case where both i' and j' are even and the case where both i' and j' are odd are the same. From the same Section B.3, the case where i' is even and j' odd is the same as the case where i' odd and j' even, but is different from the preceding one. So, there are essentially two cases to be distinguished.

B.5.1 Both i' and j' even or both i' and j' odd

$$
\begin{aligned}
\sqrt{p_{\max}^{\leftrightarrow}(i',j')} = \frac{4}{\pi^2} \sum_{p,q} \frac{1}{pq} \int_{-1/2}^{1/2} \Big(& c(p,q) \sum \cos(2\pi(i'(p-1) \pm j'(q-1))x) \\
& + c(p,q) \sum \cos(2\pi(i'(p+1) \pm j'(q+1))x) \\
& - d(p,q) \sum \cos(2\pi(i'(p-1) \pm j'(q+1))x) \\
& - d(p,q) \sum \cos(2\pi(i'(p+1) \pm j'(q-1))x) \Big) dx,
\end{aligned}
$$

where

$$
c(p,q) = \frac{1}{2}\left(1 + (-1)^{\frac{p+q}{2}-1}\right), \quad d(p,q) = \frac{1}{2}\left(1 + (-1)^{\frac{p+q}{2}}\right).
$$

$c(\cdot,\cdot)$ and $d(\cdot,\cdot)$ are functions taking value 0 or 1, and complementary in the sense that $c(p,q)+d(p,q)=1$. Next, we find that

$$\begin{aligned}&\sqrt{p^{\leftrightarrow}_{\max}(i',j')}\\&=\frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}\left(c(p,q)\mathbb{I}_{2\pi(i'(p-1)\pm j'(q-1))x=0}+c(p,q)\mathrm{I}_{2\pi(i'(p+1)\pm j'(q+1))x=0}\right.\\&\quad\left.-\,d(p,q)\mathrm{I}_{2\pi(i'(p-1)\pm j'(q+1))x=0}-d(p,q)\mathrm{I}_{2\pi(i'(p+1)\pm j'(q-1))x=0}\right),\end{aligned}$$

where

$$\mathbf{i}'=\frac{i'}{\gcd(i',j')},\quad \mathbf{j}'=\frac{j'}{\gcd(i',j')}.$$

Observe that $\mathbf{i}'$, $\mathbf{j}'$ are relatively prime; hence they could not be both even. The developments follow closely the semi-infinite chain case, except that, here, $\mathbf{i}'$ and $\mathbf{j}'$ are not restricted to be positive. Hence we have to consider several cases:

B.5.1.1 $\mathbf{i}',\mathbf{j}'\geq 1$

The following is easily observed:

$$\begin{aligned}\sum_{p,q=1,3,\ldots}\frac{c(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p-1)-\mathbf{j}'(q-1)=0}(p,q)&=\sum_{m=0,2,\ldots}\frac{c(m\mathbf{j}'+1,m\mathbf{i}'+1)}{(m\mathbf{j}'+1)(m\mathbf{i}'+1)},\\\sum_{p,q=1,3,\ldots}\frac{c(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p-1)+\mathbf{j}'(q-1)=0}(p,q)&=c(1,1),\\\sum_{p,q=1,3,\ldots}\frac{c(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p+1)+\mathbf{j}'(q+1)=0}(p,q)&=0,\\\sum_{p,q=1,3,\ldots}\frac{c(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p+1)-\mathbf{j}'(q+1)=0}(p,q)&=\sum_{m=2,4,\ldots}\frac{c(m\mathbf{j}'-1,m\mathbf{i}'-1)}{(m\mathbf{j}'-1)(m\mathbf{i}'-1)}.\end{aligned}$$

The situation is pretty much the same for the terms involving $d(p,q)$:

$$\begin{aligned}\sum_{p,q=1,3,\ldots}\frac{d(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p-1)-\mathbf{j}'(q+1)=0}(p,q)&=\sum_{m=2,4,\ldots}\frac{d(m\mathbf{j}'+1,m\mathbf{i}'-1)}{(m\mathbf{j}'+1)(m\mathbf{i}'-1)},\\\sum_{p,q=1,3,\ldots}\frac{d(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p-1)+\mathbf{j}'(q+1)=0}(p,q)&=0,\\\sum_{p,q=1,3,\ldots}\frac{d(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p+1)+\mathbf{j}'(q-1)=0}(p,q)&=0,\\\sum_{p,q=1,3,\ldots}\frac{d(p,q)}{pq}\mathbb{I}_{\mathbf{i}'(p+1)-\mathbf{j}'(q-1)=0}(p,q)&=\sum_{m=2,4,\ldots}\frac{d(m\mathbf{j}'-1,m\mathbf{i}'+1)}{(m\mathbf{j}'-1)(m\mathbf{i}'+1)}.\end{aligned}$$

Here we have to make a distinction between the two cases: both i' and j' odd and both i' and j' even. We start with the easy case where both i' and j' are odd.

In this case indeed, both $\mathbf{i}' \pm \mathbf{j}'$ is even. This along with m is even yields

$$\begin{aligned} c(m\mathbf{j}'+1, m\mathbf{i}'+1) &= 1, \\ c(1,1) &= 1, \\ c(m\mathbf{j}'-1, m\mathbf{i}'-1) &= 1, \\ d(m\mathbf{j}'+1, m\mathbf{i}'-1) &= 1, \\ d(m\mathbf{j}'-1, m\mathbf{i}'+1) &= 1. \end{aligned}$$

Putting everything together, we find, using partial fraction decompositions,

$$\begin{aligned} \sqrt{p_{\max}^{\leftrightarrow}(i',j')} &= \frac{4}{\pi^2}\left(2+\sum_{m=2,4,\ldots}\frac{4}{(m^2\mathbf{i}'^2-1)(m^2\mathbf{j}'^2-1)}\right) \\ &= \frac{4}{\pi^2}\left(2+\frac{4}{\mathbf{i}'^2-\mathbf{j}'^2}\sum_{m=2,4,\ldots}\left(\frac{\mathbf{j}'^2}{m^2\mathbf{j}'^2-1}-\frac{\mathbf{i}'^2}{m^2\mathbf{i}'^2-1}\right)\right). \end{aligned}$$

Finally, recall (Lemma 3) that the infinite sums can be expressed in terms of cotangents; this yields

$$\sqrt{p_{\max}^{\leftrightarrow}(i',j')} = \frac{8}{\pi^2}\left(\frac{1}{\mathbf{i}'^2-\mathbf{j}'^2}\left(\mathbf{i}'^2\left(\frac{\pi}{2\mathbf{i}'}\right)\cot\left(\frac{\pi}{2\mathbf{i}'}\right)-\mathbf{j}'^2\left(\frac{\pi}{2\mathbf{j}'}\right)\cot\left(\frac{\pi}{2\mathbf{j}'}\right)\right)\right). \tag{11}$$

The case where both i' and j' are even is more complicated. If i' and j' have the same power of 2 in their prime number factorization, then $\mathbf{i}' \pm \mathbf{j}'$ is even and the preceding formula holds. If the powers of 2 are different, then $\mathbf{i}' \pm \mathbf{j}'$ is odd and it is easily verified that

$$\left.\begin{array}{l} c(m\mathbf{j}'+1, m\mathbf{i}'+1) \\ c(m\mathbf{j}'-1, m\mathbf{i}'-1) \\ d(m\mathbf{j}'+1, m\mathbf{i}'-1) \\ d(m\mathbf{j}'-1, m\mathbf{i}'+1) \end{array}\right\} = \begin{cases} 1 & \text{for} \qquad m = 0,4,8,12,..., \\ 0 & \text{otherwise.} \end{cases}$$

With the above, we get

$$\begin{aligned} \sqrt{p_{\max}^{\leftrightarrow}(\mathbf{i}',\mathbf{j}')} &= \frac{4}{\pi^2}\left(2+\sum_{m=4,8,\ldots}\frac{1}{(m\mathbf{j}'+1)(m\mathbf{i}'-1)}+\frac{1}{(m\mathbf{j}'+1)(m\mathbf{i}'+1)}\right. \\ &\qquad \left.-\frac{1}{(m\mathbf{j}''+1)()m\mathbf{i}'-1}-\frac{1}{(m\mathbf{j}'-1)(m\mathbf{i}'+1)}\right) \\ &= \frac{4}{\pi^2}\left(2+\sum_{m=4,8,\ldots}\frac{4}{(m^2\mathbf{j}'^2-1)(m^2\mathbf{i}'^2-1)}\right) \\ &= \frac{4}{\pi^2}\left(2+\frac{4}{\mathbf{i}'^2-\mathbf{j}'^2}\sum_{m=4,8,\ldots}\left(\frac{\mathbf{j}'^2}{m^2\mathbf{j}'^2-1}-\frac{\mathbf{i}'^2}{m^2\mathbf{i}'^2-1}\right)\right). \end{aligned}$$

In order to derive a closed-form representation of the infinite series, we need the following lemma:

Lemma 4

$$\sum_{m=4,8,\ldots} \frac{1}{m^2\mathbf{i}'^2 - 1} = \frac{1}{2}\left(1 - \left(\frac{\pi}{4\mathbf{i}'}\right)\cot\left(\frac{\pi}{4\mathbf{i}'}\right)\right).$$

Proof. The proof is the same as that of Lemma 3, except that instead of setting $z = 1/2\mathbf{i}$ we set $z = 1/4\mathbf{i}'$. ∎

Using the lemma, we finally get the closed-form formula:

$$\sqrt{p^{\leftrightarrow}_{\max}(\mathbf{i}',\mathbf{j}')} = \frac{8}{\pi^2}\left(\frac{\mathbf{i}'^2}{\mathbf{i}'^2 - \mathbf{j}'^2}\left(\frac{\pi}{4\mathbf{i}'}\right)\cot\left(\frac{\pi}{4\mathbf{i}'}\right) - \frac{\mathbf{j}'^2}{\mathbf{i}'^2 - \mathbf{j}'^2}\left(\frac{\pi}{4\mathbf{j}'}\right)\cot\left(\frac{\pi}{4\mathbf{j}'}\right)\right).$$

B.5.1.2 $\mathbf{i}' < 0 < \mathbf{j}'$

The preceding formula remains valid, after replacing i' by $-i'$.

B.5.2 i' odd and j' even

From the integral representation, we get

$$\begin{aligned}
&\sqrt{p^{\leftrightarrow}_{\max}(i',j')} \\
&= \frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}\int_{-1/2}^{1/2}\Big((-1)^{\frac{p-1}{2}}c(p,q)\sum\cos(2\pi(i'(p-1)\pm j'(q-1))x) \\
&\quad - (-1)^{\frac{p-1}{2}}c(p,q)\sum\cos(2\pi(i'(p+1)\pm j'(q+1))x) \\
&\quad - (-1)^{\frac{p-1}{2}}d(p,q)\sum\cos(2\pi(i'(p-1)\pm j'(q+1))x) \\
&\quad + (-1)^{\frac{p-1}{2}}\ d(p,q)\sum\cos(2\pi(i'(p+1)\pm j'(q-1))x)\Big)\,dx.
\end{aligned}$$

Next, we find that

$$\begin{aligned}
\sqrt{p^{\leftrightarrow}_{\max}(i',j')} = \frac{4}{\pi^2}\sum_{p,q}\frac{1}{pq}\Big(&(-1)^{\frac{p-1}{2}}c(p,q)\mathbb{I}_{2\pi(i'(p-1)\pm j'(q-1))x=0} \\
&- (-1)^{\frac{p-1}{2}}c(p,q)\mathrm{I}_{2\pi(i'(p+1)\pm j'(q+1))x=0} \\
&- (-1)^{\frac{p-1}{2}}d(p,q)\mathrm{I}_{2\pi(i'(p-1)\pm j'(q+1))x=0} \\
&+(-1)^{\frac{p-1}{2}}d(p,q)\mathrm{I}_{2\pi(i'(p+1)\pm j'(q-1))x=0}\Big).
\end{aligned}$$

Despite the extra difficulties created by the $c(\cdot,\cdot)$ and $d(\cdot,\cdot)$ functions and the various signs, the pattern remains the same as before: the indicators are nonvanishing only if

$$p = m\mathbf{j}' \pm 1, \quad q = \mathbf{i}' \pm 1$$

for some even m.

B.5.2.1 $\mathbf{i}', \mathbf{j}' > 0$

Since i' is odd and j' is even, $\gcd(i', j')$ does not contain any positive power of 2 in its prime divisors; therefore, $\mathbf{i}'$ remains odd and $\mathbf{j}'$ remains even; in other words, $\mathbf{i}' + \mathbf{j}'$ is odd. From this observation, tedious but elementary manipulations lead to the following:

$$\left.\begin{array}{l} c(m\mathbf{j}'+1, m\mathbf{i}'+1) \\ c(m\mathbf{j}'-1, m\mathbf{i}'-1) \\ d(m\mathbf{j}'+1, m\mathbf{i}'-1) \\ d(m\mathbf{j}'-1, m\mathbf{i}'+1) \end{array}\right\} = \left\{\begin{array}{lll} 1 & \text{for} & m = 0, 4, 8, 12, ..., \\ 0 & \text{otherwise.} & \end{array}\right.$$

Next, tedious but elementary manipulation reveal that

$$(-1)^{\frac{p-1}{2}} = \left\{\begin{array}{lll} 1 & \text{if} & p = m\mathbf{j}'+1, \\ 0 & \text{if} & p = m\mathbf{j}'-1. \end{array}\right.$$

Putting everything together yields

$$\begin{aligned} \sqrt{p^{\leftrightarrow}_{\max}(\mathbf{i}', \mathbf{j}')} &= \frac{4}{\pi^2}\left(2 + \sum_{m=4,8,...} \frac{1}{(m\mathbf{j}'+1)(m\mathbf{i}'-1)} + \frac{1}{(m\mathbf{j}'+1)(m\mathbf{i}'+1)} \right. \\ &\qquad \left. - \frac{1}{(m\mathbf{j}''+1)()m\mathbf{i}'-1} - \frac{1}{(m\mathbf{j}'-1)(m\mathbf{i}'+1)}\right) \\ &= \frac{4}{\pi^2}\left(2 + \sum_{m=4,8,...} \frac{4}{(m^2\mathbf{j}'^2-1)(m^2\mathbf{i}'^2-1)}\right) \\ &= \frac{4}{\pi^2}\left(2 + \frac{4}{\mathbf{i}'^2 - \mathbf{j}'^2} \sum_{m=4,8,...} \left(\frac{\mathbf{j}'^2}{m^2\mathbf{j}'^2-1} - \frac{\mathbf{i}'^2}{m^2\mathbf{i}'^2-1}\right)\right). \end{aligned}$$

In order to derive the closed form solution, we invoke Lemma 4 and find that

$$\sqrt{p^{\leftrightarrow}_{\max}(\mathbf{i}', \mathbf{j}')} = \frac{8}{\pi^2}\left(\frac{\mathbf{i}'^2}{\mathbf{i}'^2 - \mathbf{j}'^2}\left(\frac{\pi}{4\mathbf{i}'}\right)\cot\left(\frac{\pi}{4\mathbf{i}'}\right) - \frac{\mathbf{j}'^2}{\mathbf{i}'^2 - \mathbf{j}'^2}\left(\frac{\pi}{4\mathbf{j}'}\right)\cot\left(\frac{\pi}{4\mathbf{j}'}\right)\right).$$

B.5.2.2 $\mathbf{i}' < 0 < \mathbf{j}'$

Again the preceding formula remains valid after replacing i' by $-i'$.

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