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LETTER TO THE EDITOR

Anomalous thermal conductivity and local temperature distribution on harmonic Fibonacci chains

Masashi Torikai and Takashi Odagaki

Department of Physics, Kyushu University, Fukuoka 812-8581, Japan

E-mail: M.Torikai@cmt.phys.kyushu-u.ac.jp

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Abstract
The validity of the Fourier law of heat conduction is examined for the harmonic Fibonacci chain, which has a singular continuous frequency spectrum and critical eigenstates. It is shown that the heat current J depends on the system size N as $J \sim (\ln N)^{-1}$ and the local temperature strongly oscillates along the chain. These results indicate that the Fourier law does not hold on the harmonic Fibonacci chain. Furthermore, it is shown that the local temperature exhibits two different distributions according to the generation number of the Fibonacci chain, i.e., the local temperature distribution does not have a definite form in the thermodynamic limit. The relations between the N-dependence of J and the frequency spectrum, and between the local temperature and critical eigenstates are discussed.

Many studies in recent decades have shown that arbitrarily defined one-dimensional (1D) systems of interacting particles do not exhibit normal thermal transport properties, i.e., the Fourier law does not hold for such systems [1–6]. For the steady state of the homogeneous 1D chain of system size N, the Fourier law, $J = -\kappa \nabla T$ with thermal conductivity κ, indicates that the heat current depends on the system size as $J \sim 1/N$ and that the temperature gradient ∇T is constant along the chain. Rieder *et al* [1] have shown for a 1D chain of equal-mass particles interacting with identical harmonic potentials that the heat current is independent of the system size. They also have obtained the local temperature distribution. The local temperature behaves in an unphysical way: the temperature takes a constant value in the bulk. Furthermore, near the end of the chain, the temperature decreases as we move in the direction of the hotter heat bath, and rises only at the end particle in contact with the heat bath; the temperature exhibits corresponding behaviour at the other end of the chain. Casher and Lebowitz [2] have shown for the same model but with random mass distribution that $J \sim N^{-3/2}$. For the same random-mass-distribution model but with different types of heat bath, Rubin and Greer [3] have obtained the result $J \sim N^{-1/2}$. These system size dependences of J for periodic or disordered chains may be attributed to the localization property of eigenstates on these chains. Since the eigenstates are extended in periodic chains, the ballistic energy transport of extended eigenstates results in a constant heat current of the periodic chains. In contrast, for the disordered chains, the decrease in the heat current with increasing system size is caused by the localized eigenstates, which cannot transport energy over the length of the system. The extended and localized eigenstates correspond to continuous and pure-point spectra, respectively. It is shown that, for the Casher and Lebowitz type of chain and heat bath, the thermal conductivity κ diverges as the system size increases if the spectrum contains an absolutely continuous part [2].

Some quasiperiodic systems have a Cantor-set-like spectrum, i.e., a singular continuous spectrum [7–11]. In such systems, there are eigenstates which are neither localized nor exponentially localized. For example, the Fibonacci chain, which is a 1D harmonic chain in which the spring constants and/or mass of particles are arranged according to the Fibonacci sequence, has a singular continuous spectrum [7–10]. In the Fibonacci chain, the low-frequency eigenstates are extended but the medium- and high-frequency eigenstates show power law decay (such eigenstates with power law decay are called critical states [11]). We may thus expect such quasiperiodic systems to show exotic heat transport properties compared with periodic or disordered systems.

In the present letter we investigate the anomalies of heat transport phenomena on harmonic Fibonacci chains. We focus on the anomaly resulting from the spectral properties of the Fibonacci chain. In order to check the validity of the Fourier law on the Fibonacci chain, we investigate the system size dependence of the heat current J. Although Maciá [12] has already studied the thermal conductivity κ of the harmonic Fibonacci chain, he has not checked the system size dependence of κ and thus the validity of the Fourier law is not clear yet. Our results show that the heat current behaves as $J \sim (\ln N)^{-1}$, which is in contrast with the behaviour for periodic or disordered chains. We discuss the fact that the total bandwidth of the phonon spectrum of the Fibonacci chain has similar N-dependence to J. We also calculate the local temperature distribution on the Fibonacci chain; it seems not to converge to a definite form even in the thermodynamic limit. We relate $\{T_i\}$ to the critical eigenstates of the Fibonacci chain.

The harmonic Fibonacci chain which we consider is a 1D chain of N particles; each particle interacts with its neighbouring particles with equal spring constant k. We construct the sequence of masses of particles $\{m_i | i = 1, \ldots, N; m_i = m_\alpha \text{ or } m_\beta\}$ according to the Fibonacci sequence. The Fibonacci sequence of the nth generation L_n, which consists of two kinds of component m_α and m_β, is constructed using the recursion relation $L_n = L_{n-1}L_{n-2}$, with $L_0 = m_\beta$ and $L_1 = m_\alpha$. Then the system size of the nth-generation Fibonacci sequence is the Fibonacci number F_n, which obeys the recursion relation $F_n = F_{n-1} + F_{n-2}$, with $F_0 = 1$ and $F_1 = 1$. The Fibonacci number F_n behaves asymptotically as $F_n \sim \tau^n$ (with the golden ratio $\tau = (\sqrt{5} + 1)/2$). We can obtain the asymptotic properties of the Fibonacci chain in the limit of $N \to \infty$ by considering the infinite-generation limit $n \to \infty$. We set both the spring constant k and the mass m_β to unity; we calculate the heat current and the temperature distribution varying the mass m_α.

We consider the following Langevin equations for particles of the chain with stochastic heat baths at both ends:

$$\begin{aligned} m_1\ddot{x}_1 &= -2x_1 + x_2 - \gamma\dot{x}_1 + \eta_{\mathrm{L}}(t), \\ m_i\ddot{x}_i &= -2x_i + x_{i-1} + x_{i+1}, \\ m_N\ddot{x}_N &= -2x_N + x_{N-1} - \gamma\dot{x}_N + \eta_{\mathrm{R}}(t), \end{aligned} \tag{1}$$

where x_i are the displacements of the particles from their equilibrium positions; γ is the friction constant; η_{L} and η_{R} are the random forces caused from left and right heat baths, respectively.

We choose as the random forces white noises (Casher–Lebowitz-type heat bath [2, 4]), i.e., the Fourier transforms of the random force obey

$$\begin{aligned}\langle\eta_{\rm L}(\omega)\eta_{\rm L}(\omega')\rangle &= 4\pi\gamma T_{\rm L}\delta(\omega+\omega'),\\ \langle\eta_{\rm R}(\omega)\eta_{\rm R}(\omega')\rangle &= 4\pi\gamma T_{\rm R}\delta(\omega+\omega'),\end{aligned} \tag{2}$$

where angular brackets indicate averages over the random force; $T_{\rm L}$ and $T_{\rm R}$ are the temperatures of the left and right heat baths, respectively.

We define the energy current J_i from site i to site $i+1$ as

$$J_i = \tfrac{1}{2}\langle(\dot{x}_{i+1}+\dot{x}_i)(x_{i+1}-x_i)\rangle. \tag{3}$$

We choose the definition of $\{J_i\}$ to satisfy the equation of continuity for the local energies e_i: $\dot{e}_i = -J_i + J_{i-1}$, where we have defined the local energy of the ith site as

$$e_i = \langle\tfrac{1}{2}m_i\dot{x}_i{}^2 + \tfrac{1}{2}u_i\rangle, \tag{4}$$

with the local potential energy of the ith site $u_i = (x_i - x_{i-1})^2/2 + (x_{i+1}-x_i)^2/2$. In the steady state, the energy current does not depend on the site; then from the Langevin equation (1),

$$J = \Delta T\int_0^\infty \frac{{\rm d}\omega}{\pi}\,\frac{2\gamma^2\omega^2}{|\det Y|^2}, \tag{5}$$

where $\Delta T = T_{\rm L} - T_{\rm R}$ and $Y = \Phi - \omega^2 M + {\rm i}\omega\Gamma$ with $\Phi_{ij} = -\delta_{i,j-1} + 2\delta_{ij} - \delta_{i,j+1}$, $M_{ij} = m_i\delta_{ij}$, and $\Gamma_{ij} = \gamma(\delta_{i,1}+\delta_{i,N})\delta_{i,j}$. We may write

$$\det Y = D_{1,N} - \gamma^2\omega^2 D_{2,N-1} + {\rm i}\gamma\omega(D_{2,N} + D_{1,N-1}), \tag{6}$$

where $D_{i,j}$ denotes the determinant of the sub-matrix of $\Phi - \omega^2 M$ which begins with ith row and column and ends with jth row and column [4].

We define the local temperature at site i:

$$T_i = \left\langle p_i\frac{\partial H}{\partial p_i}\right\rangle = \left\langle\frac{p_i{}^2}{m_i}\right\rangle, \tag{7}$$

where H is the Hamiltonian of the system. We note that the equipartition relation $T_i = \langle x_i\,\partial H/\partial x_i\rangle$ holds for any mass distribution (for the periodic case, the equipartition relation was proven in [1]). For our model we can write the explicit form of the local temperature as

$$T_i = T_{\rm L} - m_i\gamma\,\Delta T\int_{-\infty}^\infty \frac{{\rm d}\omega}{\pi}\,\omega^2\left|\frac{D_{1,i-1} + {\rm i}\gamma\omega D_{2,i-1}}{\det Y}\right|^2. \tag{8}$$

In calculating the heat current, it is convenient to express the determinant $D_{i,j}$ in terms of a transfer matrix as

$$\begin{pmatrix} D_{i,j} & -D_{i+1,j}\\ D_{i,j-1} & -D_{i+1,j-1}\end{pmatrix} = M_j M_{j-1}\cdots M_{i+1}M_i, \tag{9}$$

where the matrix $M_i(\omega)$ is the unimodular transfer matrix of site i defined as

$$M_i(\omega) = \begin{pmatrix} 2 - m_i\omega^2 & -1\\ 1 & 0\end{pmatrix}. \tag{10}$$

If we rewrite the total transfer matrices of the nth-generation Fibonacci chains as $\mathcal{M}_n = M_N M_{N-1}\cdots M_1$ with $N = F_n$, then the $\mathcal{M}_n$ obey a recursion relation:

$$\mathcal{M}_n = \mathcal{M}_{n-2}\mathcal{M}_{n-1}, \qquad \text{where } \mathcal{M}_0 = \begin{pmatrix} 2 - m_\beta\omega^2 & -1\\ 1 & 0\end{pmatrix} \text{ and } \mathcal{M}_1 = M_1. \tag{11}$$

Since we can obtain all the determinants $D_{i,j}$ needed in (6) by calculating $\mathcal{M}_n$, the recursion relation (11) saves a lot of time in calculating J.

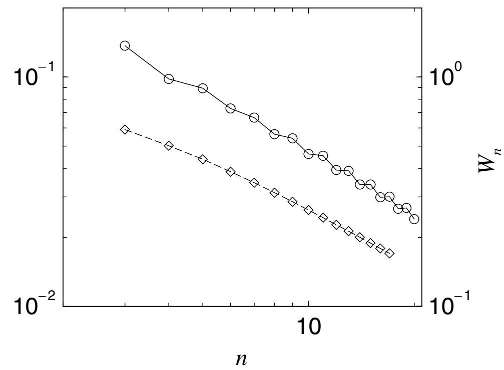

Figure 1. A log–log plot of the generation number n versus the heat current J (circles) and the total bandwidth W_n (diamonds). Curves are included to guide the eye. The masses of particles in the Fibonacci chain are $m_\alpha = 1.9$ and $m_\beta = 1.0$. The total bandwidth W_n is normalized by the maximum eigenfrequency.

We calculated the heat current and the local temperature by numerical integration of (5) and (8), respectively. As the system size grows larger, and as the mass ratio m_α/m_β becomes further from unity, the integrands of (5) and (8) vary more rapidly; hence we should use finer intervals in the numerical integration. For all the following data on J and $\{T_i\}$, we checked that decreasing the intervals of integration by a factor of 5 did not make significant changes to the results.

From the numerical calculation, we found that the total energy current J decreases with oscillation as the generation number n increases (see figure 1). The decrease of J for generation n shows power law behaviour $J \sim n^{-a}$; the exponent is $a \sim 1$ for sufficiently large m_α (e.g., $a = 1.03$ when $m_\alpha = 3.0$). This result indicates that it is appropriate to discuss the heat current in terms of the generation number n rather than the system size N. We note that the system size dependence $J \sim n^{-a} \sim (\ln N)^{-a}$ is remarkably different from the behaviour $J \sim N^{-b}$ of periodic or disordered systems.

In order to discuss the contribution of eigenstates of the chain to the total heat current we calculate, as was done in [12], the cumulative heat current:

$$J_c(\omega) = \Delta T \int_0^\omega \frac{d\omega'}{\pi} \frac{2\gamma^2\omega'^2}{|\det Y|^2}. \tag{12}$$

The cumulative heat current $J_c(\omega)$ is a monotonically increasing function; the increment of $J_c(\omega)$ in a certain ω-region is the contribution of the eigenstates of the ω-region to the total heat current. For the Fibonacci chain, as shown in figure 2, $J_c(\omega)$ consists of many slopes and plateaus. Each slope consists of slopes and plateaus in a nested fashion, and the nested structure becomes finer as the generation number grows; i.e., $J_c(\omega)$ seems to become the devil's staircase in the infinite-generation limit.

The devil's-staircase-like structure of $J_c(\omega)$ is very similar to the integrated density of states (IDOS) of the Fibonacci chain (see figure 2). The plateaus of $J_c(\omega)$ approximately coincide with the plateaus of the IDOS; i.e., the frequencies corresponding to the eigenstates make a major contribution to the heat current.

Figure 2 shows that dominant contribution to J comes from the low-frequency eigenstates, especially for high generation number. We may attribute the high conductivity in the low-frequency region to the extended eigenstates. The high-frequency eigenstates are critical, i.e., they show a power law decay, while the low-frequency eigenstates are extended like eigenstates

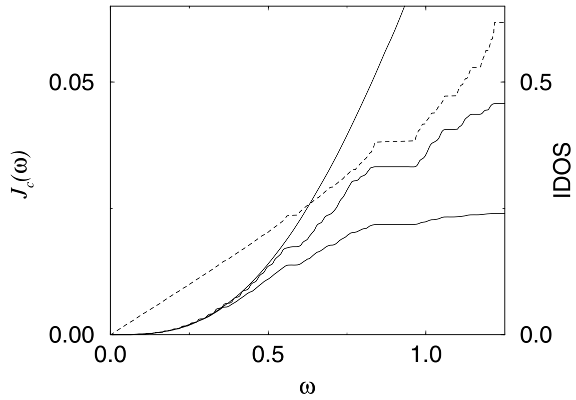

Figure 2. Full curves indicate the cumulative heat currents $J_c(\omega)$. The lower two full curves are $J_c(\omega)$ of 10th-generation (upper curve) and 20th-generation (lower curve) Fibonacci chains with $m_\alpha = 1.9$ and $m_\beta = 1.0$. The uppermost smooth full curve is $J_c(\omega)$ for a periodic chain with identical particles; the mass of particles is the average of those of the particles in the above two Fibonacci chains. The dashed curve is the IDOS of the 15th-generation Fibonacci chain. Although there are eigenstates in the high-frequency region (up to $\omega \sim 1.7$), we plot only low- and medium-frequency regions because high-frequency states contribute little to $J_c(\omega)$.

in periodic chains. Correspondingly, the low-frequency eigenstates may transport the energy ballistically. The ballistic transport can be seen from the similarity between $J_c(\omega)$ for the Fibonacci chain and $J_c(\omega)$ for a periodic chain in a low-frequency region (see figure 2). We should note that the low-frequency region in which the eigenstates are extended becomes narrower in the limit of infinite system size. This is because all the eigenstates become critical in the limit of infinite system size, since the continuous part of the spectrum of the Fibonacci chain narrows and becomes singular continuous even in the low-frequency region [7]. As a consequence, we can conclude that the heat current, unlike that of the periodic chain, vanishes when $N \to \infty$.

The similarity between $J_c(\omega)$ and the IDOS indicates that the generation number dependence of J is explained by the spectral properties of the Fibonacci chain. Now, we consider the nth-generation rational approximant, which is a periodic chain whose unit cell is the nth-generation Fibonacci chain. We denote by σ_n the ω^2-spectrum of the nth-generation rational approximant; σ_n is given as $\{\omega^2; |\mathrm{tr}\,\mathcal{M}_n| \leqslant 2\}$. The spectrum σ_n consists of F_n bands; as n increases, the bands are fragmented into pieces and total bandwidth W_n decreases. We note that W_n obeys a power law $W_n \sim n^{-a'}$ and $a' \sim 1$ [7]. Since the frequency region corresponding to the band gap does not contribute to the heat current, we conclude that the decay of J with increasing n is similar to the decay of W_n; thus J obeys a power law as W_n does, as shown in figure 1.

Unlike our result, that of Bafaluy and Rubí [13] shows that the heat current on a homogeneous harmonic chain is proportional to the total bandwidth of the ω-spectrum (instead of the ω^2-spectrum) of the chain. The difference in the bandwidth dependence of the heat current is caused not only by the difference in mass distribution of the chains but also by the choice of the heat baths. Bafaluy and Rubí did not use a white-noise heat bath; they studied a stationary state achieved from an initial state in which both the left and right half-infinite parts of the chain are in equilibrium at temperatures T_L and T_R, respectively. As shown by Dhar [4], the system size dependence of the heat current on disordered harmonic chains sensitively depends on the choice of the heat baths. We shall report on the system size dependence of the heat current for other heat baths in a future publication.

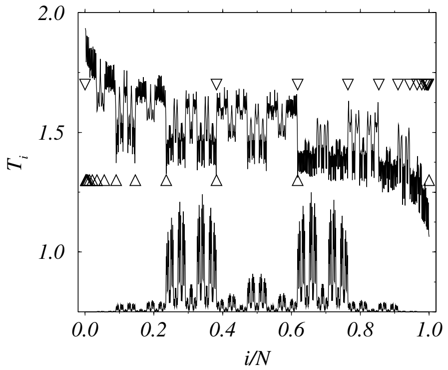

Figure 3. The upper full trace is local temperature $\{T_i\}$ on the 15th-generation Fibonacci chain with $m_\alpha = 1.9$ and $m_\beta = 1.0$. Left and right heat baths have temperature $T_\mathrm{L} = 2.0$ and $T_\mathrm{R} = 1.0$, respectively. Triangles indicate the Fibonacci sites: upward- and downward-pointing triangles correspond to the F_jth and $(F_{15} - F_j)$th sites, respectively. The lower full trace is $m_i x_i^2(\omega)$ for a critical eigenstate corresponding to the maximum eigenfrequency.

Before showing the local temperature $\{T_i\}$, we define Fibonacci sites and Fibonacci blocks, which seem important for discussing the behaviour of $\{T_i\}$. On the nth-generation Fibonacci chain, which consists of F_n sites, the Fibonacci site is the F_jth site with $j = 1, 2, \ldots, n-1$ from left or right ends; i.e., the Fibonacci sites are numbered F_j or $F_n - F_j$. We call a region between neighbouring Fibonacci sites a Fibonacci block. Since $F_j \sim \tau^j$, Fibonacci sites are sparsely distributed around the centre of the chain and densely near the ends. If the chain length is normalized to unity, the Fibonacci sites are approximately at τ^{-j} and $1 - \tau^{-j}$. Thus, as the generation number increases, the Fibonacci site distribution becomes denser near the ends but is invariant around the centre of the chain. Correspondingly, the size of the Fibonacci blocks around the centre of the chain stays constant with increasing generation number.

Now we plot $\{T_i\}$ in figure 3 where we also show the Fibonacci sites. We can see that the local temperature oscillates strongly along the chain. The oscillation in the local temperature profile shows that the heat current may flow from a lower-temperature site to a higher-temperature site. (The heat current is same everywhere on the chain, since we are considering the steady state in which the local energy of every site is constant.) Such a rather unnatural property is common among harmonic chains. For example, near the lower-temperature heat bath of the harmonic chain of equal-mass particles, there is a region in which the heat current flows from a lower-temperature site to a higher-temperature site since in that region the local temperature increases on approaching the low-temperature heat bath [1]. The disordered harmonic chains also show a strong oscillation in the local temperature before averaging over some realizations of the disorder. We may say that the Fourier law does not hold locally on these chains.

Figure 3 shows that $\{T_i\}$ changes discretely almost everywhere; however, most of the significant leaps are located at Fibonacci sites. Furthermore, the interior of each Fibonacci block has a bilaterally symmetric temperature distribution. The symmetry is a nontrivial result since the whole system with heat baths at both ends is not bilaterally symmetric. We note that some of the Fibonacci blocks have a symmetric mass sequence, but not all the blocks do.

We have not yet elucidated the mechanism producing the local temperature profile which we observed. However, we note that the mass-weighted amplitudes of critical eigenstates also have leaps at the Fibonacci sites, as shown in figure 3. Such behaviour is similar to that of the $\{T_i\}$; thus we may assume that this characteristic of the $\{T_i\}$ is partly due to the critical eigenstates. We may not simply attribute the origin of the symmetry of $\{T_i\}$ in Fibonacci blocks

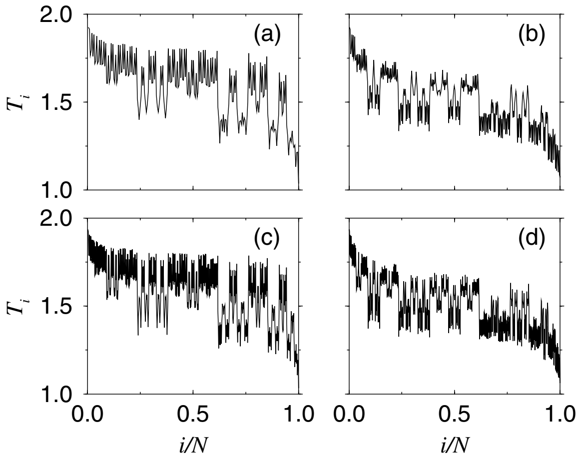

Figure 4. The local temperature on the Fibonacci chain of generation (a) $n = 12$ (number of particles $N = 233$), (b) $n = 13$ ($N = 377$), (c) $n = 14$ ($N = 610$), and (d) $n = 15$ ($N = 987$). The Fibonacci chains consist of particles of $m_\alpha = 1.9$ and $m_\beta = 1.0$. Each chain length is normalized to unity. Left and right heat baths have temperature $T_L = 2.0$ and $T_R = 1.0$, respectively.

to the properties of a single critical state, since we have not observed such symmetry in any critical states. We believe that the relation between $\{T_i\}$ and the critical eigenstates could be clarified by expressing T_i in terms of the amplitudes of the eigenstates [5], but this task is left for future research.

Another major characteristic of $\{T_i\}$ is an oscillatory behaviour with increasing generation number. We plot in figure 4 the local temperature on the Fibonacci chains of generations $n = 12$, 13, 14 and 15. There is an obvious similarity between the $\{T_i\}$ for $n = 12$ and 14, and between the $\{T_i\}$ for $n = 13$ and 15; i.e., $\{T_i\}$ oscillates periodically in generation with period two. We checked that the similarity in $\{T_i\}$ of odd- and even-generation chains is maintained throughout the generations from $n = 6$ to 15, which correspond to system sizes from $N = 13$ to 987. We may check the oscillation quantitatively by comparing the average local temperature of, e.g., the centre Fibonacci block of each chain. The average temperature of the centre Fibonacci block is distributed between 1.558 and 1.589 for odd-generation chains (from $n = 7$ to 15) and between 1.645 and 1.706 for even-generation chains (from $n = 6$ to 14). The periodic oscillation implies that the local temperature distribution $\{T_i\}$ does not converge to a definite distribution even in the limit of infinite generation number, i.e., in the thermodynamic limit.

In summary, we have shown that the Fourier law is invalid for the harmonic Fibonacci chain, as for periodic or disordered harmonic chains. The heat current J depends on the system size N as $J \sim (\ln N)^{-1}$; the anomalous dependence is remarkably different from that in the periodic or disordered case. The N-dependence of J is very similar to the N-dependence of the total bandwidth of the frequency spectrum. Such similarity is the consequence of the fact that only the lattice vibration with frequency within the frequency bands can transport the heat over the length of the chain. We have also obtained the local temperature. The local temperature $\{T_i\}$ strongly oscillates and does not show monotonic change. Both $\{T_i\}$ and the mass-weighted amplitude of the critical eigenstates exhibit significant leaps at Fibonacci sites; this fact indicates the close relation between $\{T_i\}$ and the eigenstates. We have concluded that $\{T_i\}$ does not converge to a definite form in the limit of infinite system size, since $\{T_i\}$ exhibits two different forms depending on the parity of the generation.

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