

Subdiffusive energy transport and antipersistent correlations due to the scattering of phonons and discrete breathers

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While there are many physical processes showing subdiffusion and some useful particle models for understanding the underlying mechanisms have been established, a systematic study of subdiffusive energy transport is still lacking. Here we present convincing evidence that, in the range of system size investigated, the energy subdiffusion can take place in a Hamiltonian lattice system with both harmonic nearest-neighbor and anharmonic long-range interactions. In particular, we show that the interaction range dependence of antipersistent energy-current correlations are relevant to this special type of energy subdiffusion. The underlying mechanisms are related to the various scattering processes of phonons and discrete breathers. Our results shed light on understanding the extremely slow energy transport.

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Subdiffusive motion differs from normal diffusion in that the mean squared displacement (MSD) does not grow linearly in time t , but scales as t^β with $\beta < 1$ [1]. This type of significantly slow diffusion motion was observed in many diverse complex systems, ranging from amorphous semiconductors [2] to geology [3], from weak turbulence in liquid crystals [4] to particle motion in living cells [5–7], and from the suspension of colloidal beads [8] to quantum and spin systems [9,10]. To understand the underlying mechanisms, several prominent physical models such as the confined continuous time random walk and the fractional Brownian motion were proposed [11–13]. However, most of these models were devoted to the motion of particles, the counterparts of energy transport of subdiffusion type which are ubiquitous as well, are less studied. What causes the underlying mechanisms of energy subdiffusion and how the features of energy subdiffusion emerge when dealing with a many-body Hamiltonian system are still challenging.

Due to the finiteness of the Poincaré recurrence time, it is argued that the subdiffusive motion cannot be achieved in conventional Hamiltonian systems in the absence of disorder [14]. Therefore, up to now only quite a few examples of subdiffusive energy transport in Hamiltonian systems were reported. The first convincing one is the thermal transport in a billiard channel model in a very special configuration, which shows $\beta \simeq 0.86$ [15]. However, in billiards the heat transport is performed by diffusing particles. Thus the billiard is essentially a particle model [16], in contrast to the many-body lattice Hamiltonian systems where the energy transport is conducted by phonons, i.e., the collective excitation modes or quasiparticles. This raises the interesting question of if

energy subdiffusion can exist in lattices [17]. Recently, some cues for subdiffusive energy transport, such as the vanishing of heat current, were revealed in a special Hamiltonian mean-field model [18,19]. However, some of the more significant features, such as the antipersistent [20] energy-current correlations that were frequently observed in the subdiffusion of particles, have never been explored in Hamiltonian systems. Furthermore, the origin of this antipersistence is still open.

In this Letter we first show that some features of energy subdiffusion, such as the sublinear increase of MSD in t and the subdiffusive scaling of the probability distribution function, can emerge in a many-body Hamiltonian lattice system with both harmonic nearest-neighbor (NN) and anharmonic long-range interactions (LRIs). We further explore the more convincing features of the antipersistent heat current autocorrelation. By adjusting the interaction range of the system, we reveal that the NN harmonic interaction enables the excitation of phonons, while the anharmonic LRIs, with appropriate strengths, favor the excitation of discrete breathers (DBs) [21]. These DBs can be the scatters of phonons. Therefore, various scattering processes invoke rich transports and present different antipersistence for energy subdiffusion. In this sense our result unveils new underlying physical pictures for subdiffusive motion.

We consider a one-dimensional Hamiltonian lattice of N particles under the Born–von Karman periodic boundary conditions [22] represented by

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2} + \frac{1}{2}(x_{i+1} - x_i)^2 + \frac{1}{4} \sum_{r=1}^{\tilde{N}} (x_{i+r} - x_i)^4 \right]. \quad (1)$$

Here, x_i and p_i are two canonically conjugated variables with i the index of the particle; all other relevant quantities like the particle's mass and the lattice constant are dimensionless and set to be unity. The interparticle interactions include two

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separate terms. The first one denotes the harmonic NN coupling and the second one is the anharmonic LRIs [23]. The periodic boundary conditions make our system like a ring. Similar to our previous studies [24], we do not include the Kac prefactor as that was usually performed in long-ranged systems [19]. Including this will cost that both the phonon's group velocity and the strength of nonlinearity should depend on system size, which are unwanted effects for studying energy transport.

For the LRIs we first consider the system in the presence of global interactions, i.e., $\tilde{N} = \frac{N}{2} - 1$. This setup is thus seemingly similar to that of the Hamiltonian mean-field model, but we note that the phonon dispersions for both models are quite different. In particular, the latter type of LRIs in our model, together with the harmonic NN interaction, can favor the excitation of both phonons and DBs. Therefore, even though the Hamiltonian mean-field model with both NN and LRIs always supports superdiffusive transport [19], here and fortunately, we are able to reveal the subdiffusive motion.

To capture the probability distribution function of energy diffusion in such a ring at a given temperature ($T = 0.5$ is considered), we employ the equilibrium spatiotemporal correlation function (see Refs. [24–27] for details)

$$\rho_E(m, t) = \frac{\langle \Delta E_{i+m}(t) \Delta E_i(0) \rangle}{\langle \Delta E_i(0) \Delta E_i(0) \rangle} \quad (2)$$

of the local energy $E_i = \frac{p_i^2}{2} + \frac{1}{2}(x_{i+1} - x_i)^2 + \frac{1}{4} \sum_{r=1}^{\tilde{N}} (x_{i+r} - x_i)^4$ for a canonical system. Here, due to the translational invariance, the correlation depends only on the relative distance m ; $\langle \cdot \rangle$ represents the spatiotemporal average; $\Delta E_i(t) = E_i(t) - \langle E \rangle$.

To calculate $\rho_E(m, t)$, we set the total system size $N = 4096$, which ensures that an initial energy fluctuation located at the center can spread out at a time at least up to $t = 2000$. We use the velocity-Verlet algorithm [28] with a small time step 0.01 to evolve the system. We adopt a fast Fourier transform [29] algorithm to accelerate our computations. We utilize an ensemble of size about 8×10^9 .

Figure 1(a) depicts $\rho_E(m, t)$ for several long times showing an extremely slow spread of the local energy fluctuations $\Delta E_i(t)$, i.e., the probability distribution functions are quite localized and only cover a few lattice sites. This gives the first visual sign of subdiffusive energy transport. To further check this, Fig. 1(b) depicts the MSD $\langle r_E(t)^2 \rangle$ calculated by

$$\langle r_E(t)^2 \rangle = \sum_{m=-N/2}^{N/2} m^2 \rho_E(m, t) \quad (3)$$

of $\rho_E(m, t)$. $\langle r_E(t)^2 \rangle \sim t^{0.48}$ for a short t and $\langle r_E(t)^2 \rangle \sim t^{0.21}$ at long times are numerically fitted [30]. Interestingly, it not only confirms our above conjecture, but also suggests addition insight, i.e., double sublinear scalings of MSD at short and long times. With this finding in mind, we next check the time dependence of $\rho_E(0, t)$ in Fig. 1(c). In the framework of the random walk model, $\rho_E(0, t)$ means the probability of the energy being at initial position at some t . For normal and super energy diffusion, one expects $\rho_E(0, t) \sim t^{-\beta}$ with $\beta = \frac{1}{2}$ and $\beta > \frac{1}{2}$, respectively [1,31]. But for the subdiffusive regime observed here, remarkably our best fitting no longer follows

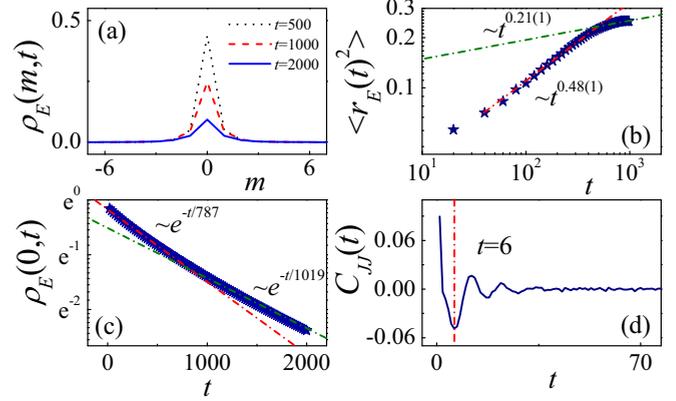


FIG. 1. Special type of subdiffusive energy transport in the system with $\tilde{N} = \frac{N}{2} - 1$: (a) $\rho_E(m, t)$ for several times t ; (b) $\langle r_E(t)^2 \rangle$ versus t showing double sublinear scalings with $\beta_1 \simeq 0.48$ and $\beta_2 \simeq 0.21$; (c) $\rho_E(0, t)$ versus t showing a two-stage exponential decay with characteristic times $\tau_1 \simeq 787$ and $\tau_2 \simeq 1019$; and (d) the equilibrium heat current autocorrelation $C_{JJ}(t)$ versus t indicating the antipersistent correlations, where the first sharp negative minimum is at $t = 6$.

a single scaling of $\rho_E(0, t) \sim t^{-\beta}$, instead it shows a manner of two-stage exponential decay $\rho_E(0, t) \sim \exp(-\frac{t}{\tau})$ with two characteristic times: $\tau_1 \simeq 787$ for short times and $\tau_2 \simeq 1019$ at long times. These two characteristic times ($\tau_1 < \tau_2$) seem consistent with the judgment of double sublinear scalings ($\beta_1 > \beta_2$) of MSD since the larger the τ , the more slowly the MSD grows.

The more convincing evidence of subdiffusion can be explored by studying the system's equilibrium heat current autocorrelation

$$C_{JJ}(t) = \langle J_{\text{tot}}(t) J_{\text{tot}}(0) \rangle, \quad (4)$$

where $J_{\text{tot}} = \sum_{i=1}^N p_i [(x_{i+1} - x_i) + \sum_{r=1}^{\tilde{N}} (x_{i+r} - x_i)^3]$ is the total heat current along the lattice. $C_{JJ}(t)$ is related to the thermal conductivity κ based on the Green-Kubo formula $\kappa = \lim_{\tau \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{k_B N T^2} \int_0^\tau C_{JJ}(t) dt$. For diffusive and superdiffusive transport, one would expect $C_{JJ} \sim \exp(-\frac{t}{\tau})$ and $C_{JJ}(t) \sim t^{-\nu}$, respectively. So κ is finite (divergent) for diffusive (superdiffusive) transport. For subdiffusive transport, however, κ should be vanishing in the thermodynamic limit, indicating the system to be a thermal insulator [16–19]. To support this, mathematically $C_{JJ}(t)$ has to change sign at least once to cause the Green-Kubo integral vanishing since it is a continuous function of t . Physically, particularly in the framework of particle models for subdiffusion [11–13], this means the property of *antipersistence*, i.e., a period of energy transport with positive heat current, is typically followed by a period of transport with negative current. Interestingly, in Fig. 1(d) the heat current autocorrelation shows a first sharp negative minimum at $t = 6$ and a few local negative minima following behind. Beyond doubt, this antipersistence surely supports the subdiffusive motion. Even though it is similar to the antipersistent velocity autocorrelations in the particle subdiffusion [1,5,6].

Combining the above evidence, we conjecture a phonon-DBs scattering picture to understand the microscopic mechanism of this subdiffusive energy transport (for this picture

in a momentum-nonconserving Hamiltonian system with on-site potential, one can refer to Ref. [32]. For the properties of DBs in nonlinear lattices with two conserved quantities, such as the discrete nonlinear Schrödinger equation, one refers to Ref. [33]. For our system we made a vivid animation for phonon-DBs scattering in zero-temperature systems, see the Supplementary Material [34]). Indeed, the harmonic NN coupling in the Hamiltonian (1) enables the excitation of phonons (with a certain phonon dispersion). Together with this phonon dispersion, the anharmonic LRIs [19] (with appropriate strengths) favor the excitation of DBs. One might regard phonons as the main heat carriers and DBs as the viscoelastic elements [6], respectively. As the phonon waves move through DBs, which is assumed as a scatterer, phonons will be partially reflected, partially pass through, and accompanied with energy loss [35,36]. The antipersistent correlations shown in Fig. 1(d) imply that the reflection takes place for short times and that DBs are finally in the majority. The double sublinear scalings ($\beta_2 < \beta_1$) of MSD [Fig. 1(b)] and the double characteristic times ($\tau_2 > \tau_1$) of $\rho_E(0, t)$ [Fig. 1(c)] thus suggest that, statistically, only a few rounds of the phonon-DBs' scattering processes play a primary role. Therefore, one might infer that the first-stage energy relaxation is induced by phonon-DBs scattering while the second-stage relatively slow relaxation is mainly caused by DBs.

To present evidence of the phonon-DBs' scattering picture in finite temperatures, we next consider a system with the truncated LRIs. This means that we set $\tilde{N} < \frac{N}{2} - 1$. This setup will weaken the strength of DBs and make the phonon-DBs' scattering more evident. This is indeed indicated in Supplementary Material [34]. However, to show DBs in finite temperatures is more challenging, and we study the spatiotemporal evolutions of local energy densities $E_i(t)$ under the equilibrium state to achieve this [24]. To do this, the ring is first thermalized to $T = 0.5$, then the thermal baths are removed and the results are recorded and displayed for a time scale $t = 1000$ by a suitable time step $\Delta t = 10$. To avoid huge data to display, we now consider a short ring of $N = 512$ instead. Figure 2 depicts the spatiotemporal evolutions of the systems with $\tilde{N} = \frac{N}{2} - 1$ and several \tilde{N} . As indicated, the DBs represented by localizations for $\tilde{N} = \frac{N}{2} - 1$ are obviously stronger than those in the truncated LRIs [see Figs. 2(a) and 2(b)]. In addition, with the decrease of \tilde{N} , the phonon-DBs' scattering leads DBs to be less evident and thus the spatiotemporal evolutions seem to show a mixed picture [see Fig. 2(c)]. Finally, if \tilde{N} is further decreased to $\tilde{N} = 1$, i.e., a system with NN couplings only, we can clearly identify the signatures of moving excitations [see Fig. 2(d)]. These excitations correspond to the long wavelength phonons or solitary waves, which are usually regarded as the microscopic origin of the superdiffusive thermal transport in the short-range interacting systems. So we here reveal that, even in the finite-temperature systems, the competition between the harmonic NN couplings and the anharmonic LRIs is important to the scattering of phonons and DBs.

More evidence of phonon-DBs' scattering in finite temperatures can be revealed by studying the typical spectrum $P(\omega)$ of the thermal fluctuations. This is achieved

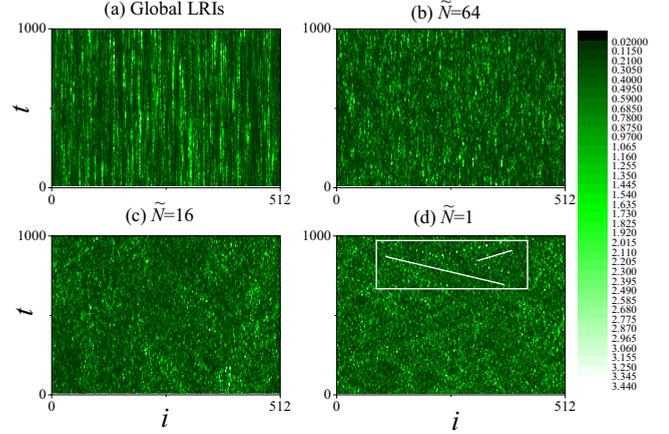


FIG. 2. DBs in finite temperatures: Spatiotemporal evolution of energy densities $E_i(t)$ for the system ($N = 512$) at thermal equilibrium for a timescale $t = 1000$ with a time step $\Delta t = 10$: (a) the global LRIs ($\tilde{N} = \frac{N}{2} - 1$); (b)–(d) the truncated LRIs with $\tilde{N} = 64$, $\tilde{N} = 16$, and $\tilde{N} = 1$ (the NN coupling case), respectively. Those marked regimes in (d) denote the mobile excitations.

by performing a frequency ω analysis of the equilibrium one particle momentum $p_{\frac{N}{2}}(t)$ along the ring: $P(\omega) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau p_{\frac{N}{2}}(t) \exp(-j\omega t) dt$ [37], where $j^2 = -1$. Figure 3 depicts $P(\omega)$ for the same setups as Fig. 2. To distinguish the long wavelength phonon waves, we adopt a log-log plot to show the low frequency components clearly. First, for a large-enough \tilde{N} , most of the frequency components are lying in above the Brillouin zone $\omega = 2$ of linear phonons, confirming the properties of DBs [see Figs. 3(a) and 3(b)]. Second, it is known that in lattices with only NN couplings supporting superdiffusive transport, the low frequency phonons are weakly damped due to the conservative feature of momentum [38,39]. As the NN anharmonicity increases we always see the damping of phonons starting from the high frequency components. This is indeed indicated in Fig. 3(d) where the low frequency can be clearly identified (see also Ref. [38]). But

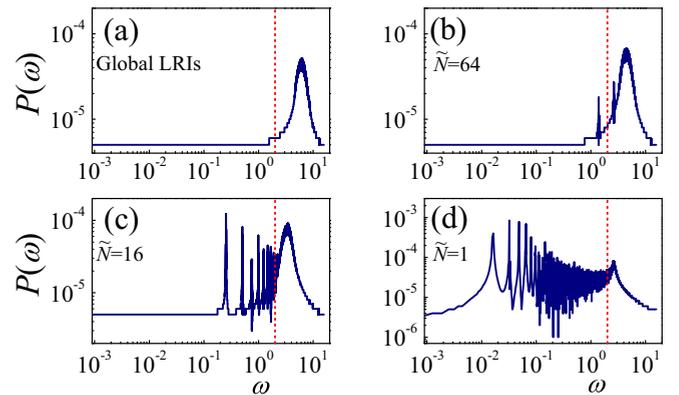


FIG. 3. Phonon-DBs' scattering in finite temperatures. The spectra $P(\omega)$ of the thermal fluctuations ($N = 512$): (a) the global LRIs ($\tilde{N} = \frac{N}{2} - 1$); (b)–(d) the truncated LRIs with $\tilde{N} = 64$, $\tilde{N} = 16$, and $\tilde{N} = 1$ (the NN coupling case), respectively. The vertical dashed lines indicate the Brillouin zone $\omega = 2$ of linear phonons.

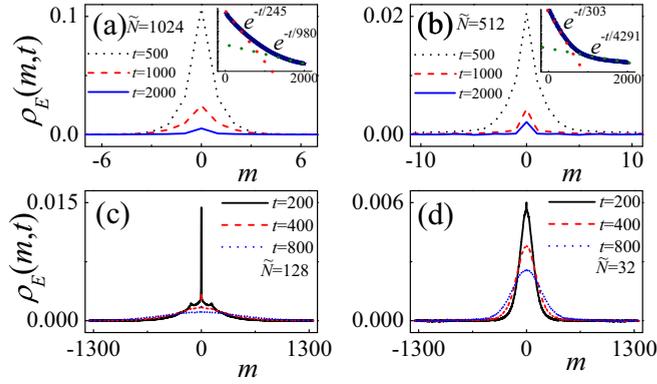


FIG. 4. From subdiffusion to superdiffusion. $\rho_E(m, t)$ for several times t for the systems with the truncated LRIs: (a) $\tilde{N} = 1024$; (b) $\tilde{N} = 512$; (c) $\tilde{N} = 128$; and (d) $\tilde{N} = 32$, respectively ($N = 4096$). The insets in (a) and (b) show $\rho_E(0, t)$ versus t . Note that the scale of the x axis is different for each panel.

after introducing the anharmonic LRIs, the situation reverses, i.e., as the anharmonicity increases we always see the attenuation of phonons beginning at the low frequency components [see Figs. 3(b) and 3(c)], and finally phonons are immersed in the environment of DBs [see Fig. 3(a)]. This later property seems to demonstrate the peculiarity of energy subdiffusion in lattices. It seems consistent with the phonon-DBs' scattering picture.

We now capture the two-stage energy relaxation and the antipersistent correlations in more detail. Toward that end, we return to the results of $\rho_E(m, t)$ and $C_{JJ}(t)$, but for the systems with the truncated LRIs instead. From Fig. 4 one expects that, for a relatively short \tilde{N} , phonons will succeed over DBs after the scattering, so the energy subdiffusion represented by $\rho_E(m, t)$ would not be seen [see Figs. 4(c) and 4(d)]. While for a relative large \tilde{N} , DBs are in the majority after the scattering, the subdiffusion can thus take place [see Figs. 4(a) and 4(b)]. Interestingly, for all the subdiffusion observed here, $\rho_E(0, t)$ always shows a two-stage relaxation [see the insets of Figs. 4(a) and 4(b)]. Therefore, whether DBs finally survive most after the scattering is crucial to the emergence of subdiffusive energy transport, and if yes the double-scaled subdiffusive motions seem always to happen.

The antipersistent correlations are still shown in the systems with the truncated LRIs [see Fig. 5]. If $\tilde{N} \geq 32$, this antipersistence will always present in our system at a universal short time $t = 6$. But, compared with the systems with the global LRIs, it turns from a sharp negative minimum to a positive dip. At present we do not know whether this is an intrinsic property of such types of systems. However, the universality of $t = 6$ shown in the systems must imply its same origin from the phonon-DBs' scattering. The only distinction is that some kinds of phonon-DBs' scattering is strong, leading to the sharp negative minimum (see Fig. 1(d) and Supplementary Material [34]); while other kinds of phonon-DBs' scattering is relatively weak and the antipersistence only presents as a dip (see Figs. 5(a) to 5(c) and Supplementary Material [34]). Another important piece of information is that $C_{JJ}(t)$ in Figs. 5(a) and 5(b) show a second antipersistence with negative minima, but these minima are not presented in Figs. 5(c) and 5(d).

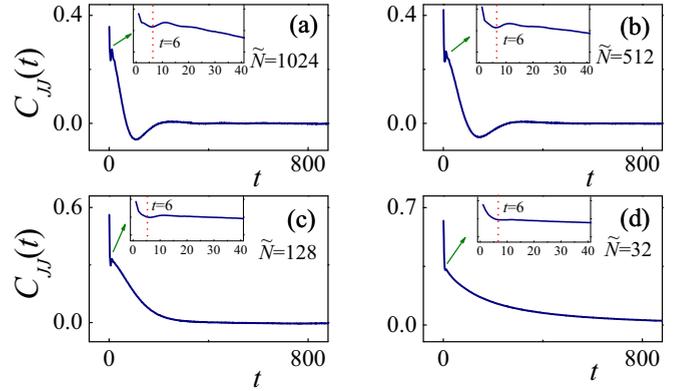


FIG. 5. The details of antipersistence. The equilibrium heat current autocorrelation $C_{JJ}(t)$ versus t for the systems with the truncated LRIs: (a) $\tilde{N} = 1024$; (b) $\tilde{N} = 512$; (c) $\tilde{N} = 128$; and (d) $\tilde{N} = 32$, respectively ($N = 4096$). The insets are a zoom for identifying the first turning point $t = 6$ for denoting the antipersistence.

Combining the results of Figs. 4(c) and 4(d), one infers that whether $C_{JJ}(t)$ has negative correlations seems crucial for signaling out the subdiffusive motion. Interestingly, the two dips shown in Figs. 5(a) and 5(b) are again in accord with the few rounds of phonon-DBs' scattering pictures.

To summarize, we presented a detailed investigation of subdiffusive energy transport in a many-body Hamiltonian lattice with long-ranged interactions. In the range of system size investigated, we observed a special type of energy subdiffusion. It shows important features of the antipersistent energy-current correlations. Even though this property is quite similar to the counterparts of particles, it would undoubtedly invoke additional insight since the energy considered here also contains the information of many-body interactions. Indeed, the overall underlying physics is now related to the phonon-DBs' scattering, i.e., the collective linear and non-linear excitations, rather than the real particles performing random walks in complicated environments. Due to this, some alternative and maybe general features, such as the two-stage energy relaxation and a universal dip indicating the antipersistent correlation emerge. Inspired by this, we are able to further clarify that the negative velocity or current correlations are crucial to judge subdiffusive motion.

Apart from these insights, to find subdiffusive energy transport in Hamiltonian dynamics in itself has its theoretical significance, which would help us check the validity of the Kac lemma [14]. In addition, the thermal conductivity in such types of systems will be vanishing in the thermodynamic limit, which implies the system to be a thermal insulator. It would thus be fascinating to expect our theoretical understanding here to invoke potential applications in designing additional thermal devices.

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