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Thermal diode utilizing asymmetric contacts to heat baths

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We propose a simple thermal diode passively acting as a rectifier of heat current. The key design of the diode is the size asymmetry of the areas in contact with two distinct heat baths. The heat-conducting medium is liquid, inside of which gaslike regions are induced depending on the applied conditions. Simulating nanoscale systems of this diode, the rectification of heat current is demonstrated. If the packing density of the medium and the working regime of temperature are properly chosen, the heat current is effectively cut off when the heat bath with narrow contact is hotter, but it flows normally under opposite temperature conditions. In the former case, the gaslike region is induced in the system and it acts as a thermal insulator because it covers the entire narrow area of contact with the bath.

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The understanding of nonequilibrium phenomena such as heat conduction is a longstanding task in nonequilibrium statistical physics. A better understanding of the mechanism of heat conduction may also lead to potentially interesting applications, such as possible designs for highly functional devices for controlling heat flow. For example, models for a thermal rectifier have been proposed for the nonlinear lattice system [1–6]. Experimental implementations in nanoscale structures [7–9] and those on a macroscopic scale [10] are also studied. Thermal devices, such as heat pumps, working at the nanoscale [11–13] are also studied, and refrigerating effects are observed in thermal ratchet models [14–16].

The key mechanism of heat rectification in hetero lattice systems, in which two different types of lattice are connected, is the strong temperature dependence of the matching property between the phonon bands at the junction of the lattices [2,17]. In order to realize thermal diodes, other mechanisms are also possible. We naively expect that simpler designs of diodes will be possible if we use thermal switches such as bimetal switches (Fig. 1), which can turn the current on/off depending on the temperature conditions.

Here, we propose a design for such a thermal diode, using liquids as heat-conducting media. The key design of the diode is the size asymmetry of the areas in contact with two distinct heat baths, while the bulk of the system is composed of homogeneous particles. The gaslike phase of the system can be utilized as a simple insulator of heat. When the bath with the narrow area of contact is hotter, the area of contact with the bath is surrounded by the gaslike phase and the heat current is effectively cut off. Under the opposite temperature conditions (the bath with the wide area of contact is hotter), heat current flows normally. By nanoscale nonequilibrium molecular dynamics simulations of this system, we demonstrate that the heat rectifying (diode) effect is observed as expected. Although this model may yet be somewhat far from a realistic implementation, we nevertheless hope this Rapid Communication will lead to a possible design of practical relevance for thermal devices.

N identical particles of mass m are enclosed in a rectangular box ($L_x \times L_y \times L_z$), and two rectangular regions inside the box are set up as the areas of contact with the two heat baths attached to the system, as schematically shown in Fig. 2. Time developments of the ith particle's position $\boldsymbol{r}_i$ and momentum $\boldsymbol{p}_i$ are described as

$$(d/dt)\boldsymbol{r}_i = \boldsymbol{p}_i/m,$$

$$(d/dt)\boldsymbol{p}_i = -\sum_{j\neq i} \partial_{\boldsymbol{r}_i} V(|\boldsymbol{r}_i - \boldsymbol{r}_j|) + \boldsymbol{f}_{\text{bath}} + \boldsymbol{f}_{\text{wall}}. \quad (1)$$

Particles interact with each other through the Lennard-Jones (LJ) potential with a smoothed cutoff [18] (cut-off length $r_c = 2.5\sigma$)

$$V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6] + c_2 r^2 + c_0 \quad (2)$$

for $r < r_c$ and $V(r) = 0$ for $r \geq r_c$, where r is the distance between the particles. The parameters c_2 and c_0 are chosen so that $V(r_c) = 0$ and $(d/dr)V(r)|_{r=r_c} = 0$. We use the scale unit as $m = 1$, $\sigma = 1$, and $\epsilon = 1$.

Only when the particle is inside one of the areas of contact with the heat baths, it interacts with the heat bath through the Langevin force,

$$\boldsymbol{f}_{\text{bath}} = -\gamma_k \boldsymbol{p}_i + \sqrt{\gamma_k T_k / m}\, \boldsymbol{\xi}_k^{(i)}(t), \quad (3)$$

where $k \in \{1,2\}$ is the index of the heat bath and the temperature T_k is measured in energy units (set the Boltzmann constant as unity). The Gaussian white noise $\boldsymbol{\xi}_k(t)$ satisfies $\langle \xi_{k,u}^{(i)}(t) \xi_{k',u'}^{(i')}(t') \rangle = \delta_{ii'} \delta_{kk'} \delta_{uu'} \delta(t - t') (u \in \{x,y,z\})$. The parameters $\gamma_1 = \gamma_2 = 5$ are used for our simulation. The heat ab-

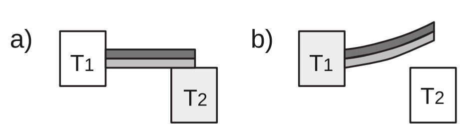

FIG. 1. Schematics of bimetal switch. The bimetal, comprising two separate metals joined together (each metal has a different thermal expansion coefficient), is fixed to the heat bath T_1 at one end. (a) When the bimetal is straight, it comes into contact with the other heat bath T_2. Then heat current can flow between the two heat baths. (b) Under some temperature conditions, the bimetal bends owing to the difference in the thermal expansion coefficients. Then there is no pathway for heat between the baths. In this way, the bimetal switch can work as an on (a) and off (b) switch for heat currents.

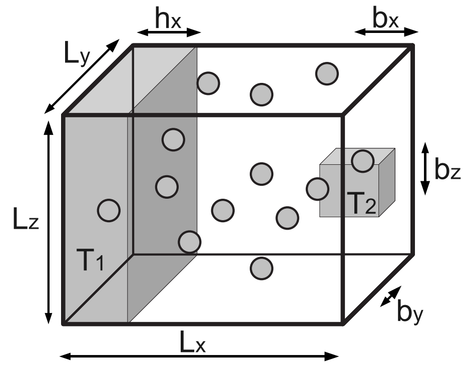

FIG. 2. Schematics of the system. N particles are enclosed in the rectangular box ($L_x \times L_y \times L_z$). They interact with each other through the LJ potential. Two gray rectangular regions inside the box are set up as the areas of contact with the heat baths (at temperatures T_1 and T_2). Only when particles are inside these regions, they are subjected to Langevin thermal forces. We introduce asymmetry in the sizes of the areas of contact with the heat baths: the area of contact with the bath 1 on the left side has the volume $h_x \times L_y \times L_z$, whereas that with the bath 2 on the right side has the smaller volume $b_x \times b_y \times b_z$. In most simulations, we used $L_x=24$, $L_y=L_z=48$, and $h_x=b_x=b_y=b_z=6$. The mirrored wall conditions are applied on both ends along the x direction and the periodic boundary conditions are applied along the other directions (y,z).

sorbed into the system from each heat bath is measured using stochastic energetics [19].

The two ends along the x direction are (mirror) wall boundaries [20], i.e., each particle near the wall is (additionally) receives force from the self-mirror image with the interaction potential $V(r)$,

$$\boldsymbol{f}_{\text{wall}} = \hat{\boldsymbol{e}}_{\text{n}} \frac{d}{dr} V(r) \Bigg|_{r=2|x_i - X_{\text{wall}}|}, \tag{4}$$

where $x_i(X_{\text{wall}})$ is the x component of the ith particle (wall) position and $\hat{\boldsymbol{e}}_{\text{n}}$ is the unit vector normal to the wall (directed from the inside to the outside of the system). Periodic boundary conditions are applied for the other two (y,z) directions.

The thermal diode effect is clearly observed, as shown in Fig. 3, where the steady heat currents are plotted for various bath temperatures. When the temperature of the narrow-contact bath 2 is sufficiently higher than that of the wide-contact bath 1 ($T_1 < T_2$), the heat current is effectively cut off, whereas normal heat conduction occurs for a wide range of parameters such that $T_1 > T_2$.

Figure 4 shows snapshots of the system (particle positions in the xy-plane slice of the thickness b_z, which includes the whole area of contact with the narrow-contact bath) in the heat-conducting steady state. When the narrow-contact bath is hotter ($T_1 < T_2$), a gaslike phase surrounds the area of contact with the bath and heat current is effectively cut off.

Figure 5 shows the response of the heat current to the switching of the temperature conditions. The system smoothly exhibits on-off switching of the heat currents in both directions of switching and works well as a thermal diode.

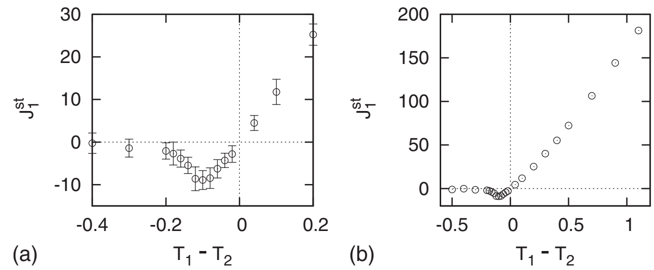

FIG. 3. Performance of the rectification of thermal current. The steady heat current J_1^{st} (energy per unit time) from bath 1 to the system, which is equal to $-J_2^{\text{st}}$ from bath 2, is plotted versus the temperature difference $T_1 - T_2$ of the baths. (a) Close-up of (b). We used the number density $\rho=0.65$ ($N=35942$) and the mean temperature $(T_1+T_2)/2=0.75$. For each simulation, initial conditions were prepared at $T_1=T_2=0.75$ and the nonequilibrium temperature condition was applied for $t \geq 0$. The heat current (averaged for each 100 time units) was observed during $2000 < t < 4000$ [three-sigma error bars are plotted in (a)].

Figure 6 shows the packing density dependence of the thermal diode effect. In a rather wide range of packing density, the system can function as a thermal diode. For very high packing densities, the diode effects appear only with larger temperature differences. In the opposite situation, for very low packing densities (not shown in the figure), the heat currents under the condition $T_1 > T_2$, where we expect normal conduction, also become cut off by the gaslike phase, and the diode function becomes less effective.

In order to elucidate the working mechanism for the present thermal diode, the relationship between the local density $\rho(\boldsymbol{r})$ and the local (kinetic) temperature $T(\boldsymbol{r})$ in the heat-conducting steady state is plotted in Fig. 7 together with the equilibrium phase diagram. In the figure, the solid lines show the coexistence curves at equilibrium. Each line indicates coexisting liquid (or gas) states for a given temperature. In equilibrium, single-phase states between these two curves are unstable and phase separation occurs. This equilibrium information is useful in considering the working mechanism.

In the case of Fig. 7(a) where the gaslike phase appears as in Fig. 4(a), the relationship between $\rho(\boldsymbol{r})$ and $T(\boldsymbol{r})$ in most of the bulk is approximately equal to that in the coexisting liq-

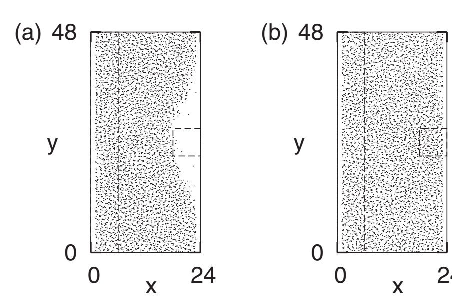

FIG. 4. Snapshot of the system in the heat conducting nonequilibrium steady states: xy coordinates of particles inside the slice of thickness $b_z=6$ are plotted with dots. The solid lines show system boundaries and the broken lines show the areas of contact with the heat baths. (a) $T_1=0.6$ and $T_2=0.9$. Gaslike regions overlap the area of contact with the narrow-contact bath. (b) $T_1=0.9$ and $T_2=0.6$. No apparent gaslike regions exist.

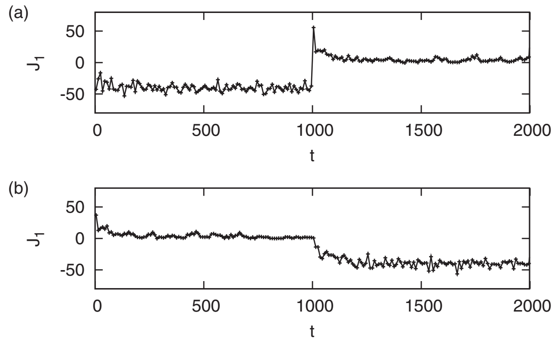

FIG. 5. Response of heat currents to switching of temperature conditions. Averaged heat currents J_1 from bath 1 (the wide-contact bath) to the system for each ten time units are plotted. Each graph shows a single trajectory of the system. Initially, the system was prepared at $T_1=T_2=0.75$. (a) At $t=0$, (T_1,T_2) is switched to (0.9, 0.6) and then to (0.6, 0.9) at $t=1000$. (b) The reverse case of (a). At $t=0$, (T_1,T_2) is switched to (0.6, 0.9) and then to (0.9, 0.6) at $t=1000$. For both directions of switching, the system exhibits smooth responses and good diode effects.

uid state at $T=0.6$. The local temperature in the interface region (data lying between the coexistence curves) connecting the bulk of liquid to the gaslike region is also approximately equal to $T=0.6$. The heat current in this nonequilibrium steady state is so small that the energy flow from the gaslike phase has little effect on the bulk of the liquid.

In the case of Fig. 7(b) where normal heat conduction occurs, the relationship between $\rho(\boldsymbol{r})$ and $T(\boldsymbol{r})$ stays within the region where the (single-phase) liquid state is stable in equilibrium. The relationship in large part of the bulk lies close to that for the liquid state at $T=0.9$.

From the above observations, it is noted that the temperatures in a large part of the bulk are approximately maintained as the same value as T_1 (the temperature of the wide-contact bath), i.e., the mean temperature of the bulk is mainly controlled by the wide-contact bath. The most essential factor for such behavior would be the size asymmetry between the contact areas of the two heat baths. Then, in the case of Fig. 7(a) the mean temperature ($\simeq 0.6$) is sufficiently low for phase separation, whereas in the case of Fig. 7(b) the mean

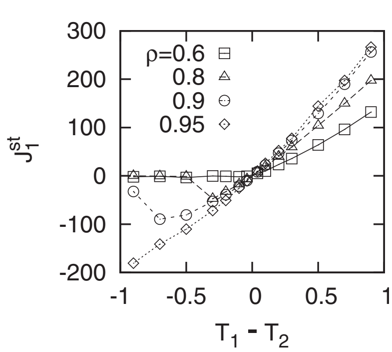

FIG. 6. Steady heat currents J_1^{st} for various number densities ρ. Almost the same setting as in the case of Fig. 3 were used. For $T_1-T_2 \geq 0.7$ and $\rho \geq 0.9$, the heat currents were observed during $5000<t<6000$. For other conditions, heat currents were observed during $1000<t<2000$.

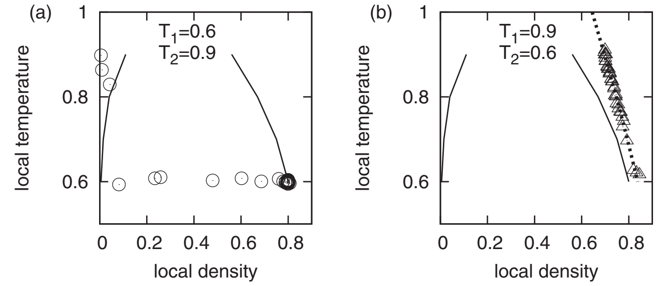

FIG. 7. Local density vs local (kinetic) temperature in the heat-conducting states (plotted with open circles or triangles). Both local quantities are averages over the particles inside the rectangular cell regions with a size of $6\times 6\times 1$ (evaluated for regions located further than 3σ from the walls). The parameters are the same as the case of Fig. 4. (a) $T_1=0.6$ and $T_2=0.9$. (b) $T_1=0.9$ and $T_2=0.6$. Solid lines are liquid-gas coexistence curves obtained by equilibrium simulations ($T_1=T_2$). Dotted line is isobar obtained by equilibrium simulations. The pressure ($p=0.48$) on the dotted line is chosen to be the same value as that in the heat-conducting steady states of (b). Data in the heat-conducting states closely follow the equilibrium line. This implies that deviations from the local equilibrium are small at the scale of this plot.

temperature ($\simeq 0.9$) is sufficiently high to maintain the system outside the coexistence region. This switching mechanism is similar to that for the bimetal switch in Fig. 1. Thus the present thermal diode works well when the packing density (and the media fluid) for the working regime is properly chosen.

In summary, we proposed a simple design for a thermal diode that utilizes the size asymmetry and gas-liquid phase of the system. Our idea is very simple: the size asymmetry introduced in the areas in contact with the heat baths leads to the diode effects. Because of the size asymmetry, the mean temperature of the bulk in the system is mainly controlled by the wide-contact heat bath. Then there is a possibility that phase separation occurs under one temperature condition whereas the system stays within the single-phase state under the opposite temperature condition. In the former case, the gaslike phase covers the region of contact with the hotter heat bath and heat current is effectively cut off. We demonstrated the function of the rectification by simulating a simple nanoscale system with our design. Such smallness of the system size may have the merit of a smooth and robust function that is free of effects of gravitational force. In the actual implementation of this design, one of the main difficulties may be in achieving a sufficiently rigid and thermally insulating container to enclose the liquid. Specific interaction between the container walls and the working fluid might also cause some difficulties. It is our hope that new engineering developments will be inspired by the simple design presented here.

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[20] We chose this boundary condition because of the convenience for the parallelized code. This choice is not essential for our results. At least, similar diode effects were observed for periodic boundary conditions in the z direction, in which the two heat baths (T_1 and T_2) are located with the separation length $L_z/2$.