# Thermal convection-diffusion crystal for prohibition and modulation of wave-like temperature profiles

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# AFFILIATIONS

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## ABSTRACT

Periodic structures have various applications in wave systems, such as atomic crystals, photonic crystals, and phononic crystals. Here, we extend the related physics from wave systems to convection-diffusion systems and propose the concept of thermal convection-diffusion crystals, referring to a periodic porous medium with moving fluid. Phenomenally speaking, only the temperature profiles with allowed frequencies can propagate stably in a thermal convection-diffusion crystal, and those with forbidden frequencies try to change their frequencies for stable propagation. As an application of thermal convection-diffusion crystals, we further design a thermal frequency modulator to manipulate wave-like temperature profiles. These results broaden the application scope of periodic structures in convection-diffusion systems and enlighten further development of thermal management and thermal metamaterials with thermal convection-diffusion crystals.

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Periodic structures have attracted widespread and lasting research interest due to their characteristics. Inspired by atomic crystals, photonic crystals<sup>1,2</sup> and phononic crystals<sup>3</sup> were proposed successively. At the micro/nanoscale, phonon is also the carrier of thermal diffusion,<sup>4</sup> and so thermocrystals<sup>5</sup> were also proposed. Periodic structures have widespread applications in designing zero-index metamaterials,<sup>6–9</sup> revealing topological properties,<sup>10–13</sup> and reducing thermal conductivities.<sup>14–16</sup>

These studies were almost conducted in wave systems because frequency and phase are two key factors. We take phononics as an example. The mechanisms of Bragg scattering<sup>3</sup> and local resonance<sup>17</sup> are closely related to the frequency and phase. However, the frequency and phase do not exist directly in convection-diffusion systems. Therefore, to date, the related physics in convection-diffusion systems is still lacking, which limits the application scope of periodic structures.

To promote the related physics, we obtain wave-like temperature profiles with the help of thermal convection. It is feasible because recent studies<sup>18,19</sup> introduced thermal convection and revealed antiparity-time symmetry in convection-diffusion systems. Another key problem is to design a thermal convection-diffusion crystal. If we follow the existing method and consider a pure material,<sup>18,19</sup> it is difficult to obtain a periodic structure. Therefore, we shift the way of thinking and study the thermal convection-diffusion process in a periodic porous medium with moving fluid (say, a thermal convectiondiffusion crystal). In this way, we obtain two key factors, say, a wavelike temperature profile and a thermal convection-diffusion crystal.

In what follows, let us start from the theory of thermal convection-diffusion crystals. The thermal convection-diffusion process in a homogeneous porous medium [see Fig. 1(a)] is dominated by

$$\partial T / \partial t + \alpha \mathbf{v} \cdot \nabla T + \nabla \cdot (-\sigma \nabla T) = 0, \tag{1}$$

where *T* and *t* denote the temperature and time, respectively,  $\alpha = \rho_f C_f / (\rho_m C_m)$ , and  $\sigma = \kappa_m / (\rho_m C_m)$ . The effective parameters of porous medium (say, density  $\rho_{m\nu}$  heat capacity  $C_{m\nu}$  and thermal conductivity  $\kappa_m$ ) can be calculated with the weighted average of solid and fluid,<sup>20</sup> namely,  $\rho_m C_m = \phi \rho_f C_f + (1 - \phi) \rho_s C_s$  and  $\kappa_m = \phi \kappa_f + (1 - \phi) \kappa_s$ .  $\rho_f$  (or  $\rho_s$ ),  $C_f$  (or  $C_s$ ), and  $\kappa_f$  (or  $\kappa_s$ ) are the density, heat capacity, and thermal conductivity of fluid (or solid), respectively.  $\phi$  is the porosity of solid.  $\boldsymbol{\nu}$  is the convective velocity of fluid, which can be generated from a pressure difference.<sup>21-25</sup> Equation (1) shows the energy conservation of thermal convection and conduction, which has both hyperbolicity (the convection term with  $\alpha \boldsymbol{\nu}$ ) and parabolicity (the diffusion term with  $\sigma$ ).



FIG. 1. Schematic diagrams. (a) Structure and (b) dispersion relation of a homogeneous porous medium composed of material I. (c) Structure and (d) forbidden rule of a periodic porous medium composed of materials I and II (say, thermal convection-diffusion crystal). Parameters are as follows:  $\rho_f = 1000 \text{ kg/m}^3$ ,  $C_f = 1000 \text{ J kg}^{-1} \text{ K}^{-1}$ ,  $\kappa_f = 0.6 \text{ W m}^{-1} \text{ K}^{-1}$ ,  $\rho_{s1} = 1000 \text{ kg/m}^3$ ,  $C_{s1} = 1000 \text{ J kg}^{-1} \text{ K}^{-1}$ ,  $\kappa_{s1} = 0.3 \text{ W m}^{-1} \text{ K}^{-1}$ ,  $\phi_1 = 1/6$ , v = 0.1 cm/s, and L = 20 cm. Subscript 1 denotes material I.

The density of fluid  $\rho_f$  does not change with time, and so mass conservation is satisfied. The convective velocity v is set to a small constant, ensuring creeping flow and momentum conservation.

For brevity, we consider a one-dimensional case with length L, and Eq. (1) becomes

$$\partial T/\partial t + \alpha v \partial T/\partial x - \sigma \partial^2 T/\partial x^2 = 0.$$
 (2)

We use a wave-like temperature profile  $T = Ae^{i(kx-\omega t)} + T_0$  whose real part makes sense,<sup>18,19</sup> and derive a dispersion relation,

$$\omega = \alpha v k - i\sigma k^2, \tag{3}$$

where  $\omega$  is the frequency, *k* is the wave number, *A* is the amplitude, and  $T_0$  is the reference temperature. The dispersion relation [Eq. (3)] shows that the convection term (with  $\alpha v$ ) results in propagation property, and the diffusion term (with  $\sigma$ ) only determines the dissipation of wave-like temperature profiles. When v = 0, a wavelike temperature profile decays without propagation because the real part of frequency  $\omega$  is zero. When  $v \neq 0$ , a wave-like temperature profile decays with propagation due to the nonzero real part of frequency  $\omega$ .

To support wave-like temperature profiles, we apply a periodic boundary condition on the left and right ends of the one-dimensional case presented in Fig. 1(a). Then, only the temperature profiles with wavelengths satisfying  $\lambda = L/N_1$  are allowed, and so wave numbers can take

$$k = 2\pi/\lambda = 2\pi N_1/L,\tag{4}$$

where  $N_1$  can be any positive integers. When *L* tends to infinity, wave numbers become continuous, thus leading to a continuous dispersion relation [see the solid lines in Fig. 1(b)]. The left (or right) axis corresponds to the real (or negative imaginary) part of frequency  $\omega$ , reflecting the propagation (or dissipation) property.

The temperature profiles satisfying the dispersion relation [Eq. (3)] can propagate smoothly in a homogeneous porous medium. However, if two porous media (material I with length  $L_1$  and material II with length  $L_2$ ) are arranged alternatively to form a thermal convection-diffusion crystal with lattice constant D = L/N [see Fig. 1(c)], yielding  $\alpha(x) = \alpha(x + D)$  and  $\sigma(x) = \sigma(x + D)$ , not all temperature profiles can propagate stably. According to the Bloch theorem, it is natural to assume that the wave-like temperature profile in a thermal convection-diffusion crystal is a plane wave with a periodic amplitude modulation, which can be expressed as

$$T = Tu(x)e^{i(kx-\omega t)} + T_0,$$
(5)

where  $u(x) = u(x + N_2D)$  is a periodic function and  $N_2$  can be any positive integers ( $N_2 \le N$ ). Obviously, the wave-like temperature profile described in Eq. (5) should also have a spatial periodicity,

$$T(x) = T(x + N_2 D).$$
 (6)

Equation (6) gives  $e^{ikN_2D} = 1$ , and so only the wave numbers satisfying  $kN_2D = 2\pi$  can survive a thermal convection-diffusion crystal,

$$k = 2\pi (1/N_2)/D = 2\pi (N/N_2)/L.$$
(7)

Comparing Eqs. (4) and (7), we can derive

$$N_1 = N/N_2, \tag{8}$$

where  $N_2$  can only take on the divisors of N for ensuring  $N_1$  to be an integer  $(N_1 \leq N)$ . In one word, wavelength must be an integer multiple of lattice constant D, and it should satisfy the requirement of the periodic boundary condition. Since not all  $N_1$  can meet the requirement, the prohibition and modulation of wave-like temperature profiles can be achieved [see Fig. 1(d)]. When  $N_1$  takes on a value denoted by the circle, the wave-like temperature profile can propagate stably in a thermal convection-diffusion crystal. However, if  $N_2$  takes on a value denoted by the cross, the wave-like temperature profile cannot propagate stably, and the related frequency is forbidden and modulated.

To confirm the theory, we perform finite-element simulations using COMSOL Multiphysics (http://www.comsol.com/). We first check the dispersion relation [Eq. (3)]. As required by the periodic boundary condition, wave numbers can only take on discrete values, whose simulation results are plotted as dots in Fig. 1(b). There are small deviations between theory and simulation because Eq. (2) is an effective equation with parameters taking the weighted average of fluid and solid.

Then, we discuss the case with N = 4 and set the same porosity of two solids. Therefore, mass conservation can be satisfied, and convective velocity is a constant. Without loss of generality, we set  $\alpha$  as a constant and  $\sigma$  to be periodic, say,  $\sigma(x) = \sigma(x+D)$ . According to the theoretical prediction [Eq. (8)],  $N_1 = 1, 2, 4$  can ensure wave-like temperature profiles to propagate stably, whereas  $N_1 = 3$  cannot. For proof, we set initial wave-like temperature profiles as T =  $30 \sin [k(x - \lambda/4)] + 310$  K, where k is determined using Eq. (4) with  $N_1 = 1, 2, 3, 4$  (see the solid lines in the left column of Fig. 2). All these wave-like temperature profiles can propagate smoothly in a homogeneous porous medium (see the dashed lines in the left column of Fig. 2). However, not all these wave-like temperature profiles can propagate stably in a thermal convection-diffusion crystal (see the dashed-dotted lines in the left column of Fig. 2). For  $N_1 = 1, 2, 4$ , the temperature profiles become plane waves with periodic amplitude modulations. For  $N_1 = 3$ , the temperature profile is forbidden, which changes its wavelength to  $N_1 = 1$ . We also plot the temperature evolution at x = 0 cm with time (see the right column of Fig. 2). The solid (or dashed) lines indicate the temperature evolution in a homogeneous (or periodic) porous medium. Clearly, time periodicity is almost unchanged for  $N_1 = 1, 2, 4$ . However, time periodicity is changed for  $N_1 = 3$  [see the dashed box in Fig. 2(f)]. Therefore, only the temperature profiles satisfying Eq. (8) are allowed to propagate stably in a thermal convection-diffusion crystal.

Furthermore, we also explore the property of forbidden wave-like temperature profiles. We discuss the case with N=8, which has four forbidden temperature profiles including  $N_1 = 3$ , 5, 6, 7. We set initial wave-like temperature profiles as  $T = 30 \sin [k(x - \lambda/4)] + 310$  K, where k is determined using Eq. (4) with  $N_1 = 3$ , 5, 6, 7 (see the solid lines in the left column of Fig. 3). The solid (or dashed) lines in the right column of Fig. 3 are the temperature evolution at x = 0 cm in a homogeneous (or periodic) porous medium. Clearly, these temperature profiles can propagate smoothly in a homogeneous medium (see the dashed lines in the left column of Fig. 3). However, the results



**FIG. 2.** Results of N = 4. Solid lines in the left column are initial temperature profiles. Dashed lines and dashed-dotted lines are the temperature profiles in a homogeneous medium and a thermal convection-conduction crystal, respectively, at (a) 1000 s, (c) 400 s, (e) 230 s, and (g) 120 s. Solid and dashed lines in the right column show the temperature evolution at x = 0 cm in a homogeneous medium and a thermal convection-conduction crystal, respectively. Parameters are as follows:  $\rho_{s2} = 1000 \text{ kg/m}^3$ ,  $C_{s2} = 1000 \text{ J kg}^{-1} \text{ K}^{-1}$ ,  $\kappa_{s2} = 9 \text{ W m}^{-1} \text{ K}^{-1}$ ,  $\phi_2 = 1/6$ , and  $L_1 = L_2 = 2.5 \text{ cm}$ . Subscript 2 denotes material II. Other parameters are the same as those in Fig. 1.

are different in a thermal convection-diffusion crystal. For  $N_1 = 3$ , its periodicity in space and time is only slightly affected [see Figs. 3(a) and 3(b)]. This is because the wavelength of  $N_1 = 3$  is much larger than the lattice constant ( $\lambda = 2.7D$ ), and the modulation effect is weakened. This explanation is in accordance with photonic crystals where the wavelength and lattice constant should be comparable. For  $N_1 = 5$ , it loses periodicity in space and time [see Figs. 3(c) and 3(d)] and cannot propagate stably. For  $N_1 = 6, 7$ , these two wave-like temperature profiles change their wavelengths to  $N_1 = 2, 1$ , respectively, in order to propagate stably [see Figs. 3(e)-3(h)]. We also provide a qualitative analysis to explain the change in wavelengths. The temperature profiles with forbidden frequencies prefer to evolve into the wavelengths with common divisors of  $N_1$  and N. For example, the common divisors of 6 and 8 are 1 and 2. 2 is closer to 6, and so  $N_1 = 6$  finally





**FIG. 3.** Results of N = 8. Solid lines in the left column are initial temperature profiles. Dashed lines and dashed-dotted lines are the temperature profiles in a homogeneous medium and a thermal convection-conduction crystal, respectively, at (a) 240 s, (c) 120 s, (e) 110 s, and (g) 140 s. Solid and dashed lines in the right column show the temperature evolution at x = 0 cm in a homogeneous medium and a thermal convection-conduction crystal, respectively. Other parameters are the same as those in Fig. 2 except for  $L_1 = L_2 = 1.25$  cm.

evolves into  $N_1 = 2$ ; the common divisor of 7 and 8 is 1, and so  $N_1 = 7$  finally evolves into  $N_1 = 1$ . It is only a qualitative analysis because it is not applicable for  $N_1 = 3$  (whose modulation effect is weakened due to its large wavelength). On all accounts, the temperature profiles with forbidden frequencies are indeed modulated by a thermal convection-diffusion crystal.

We also design an application with thermal convection-diffusion crystals (say, a thermal frequency modulator) with practical structures and parameters. The thermal modulator is a ring structure with periodicity, composed of material I (porous rock) and material II (porous metal) [see Figs. 4(a) and 4(d)]. Water flows in the ring structure with angular velocity  $\Omega$ . Since water fills the interfaces of two solids, interfacial thermal resistance<sup>26,27</sup> resulted from air can be neglected. The periodic boundary condition is naturally satisfied with the ring structure. The initial wave-like temperature profile can be obtained by heating and cooling corresponding positions. After forming a wave-like



**FIG. 4.** Thermal frequency modulator. (a) and (d) Schematic diagram. (b) and (e) Temperature profiles at t=0 s with  $N_1=2$  and  $N_1=3$ , respectively. (c) and (f) Temperature profiles at t=230 s with  $N_1=2$  and  $N_1=3$ , respectively. Color maps represent temperatures. Material I (porous rock):  $\rho_{s1}=2500$  kg/m<sup>3</sup>,  $C_{s1}=800$  J kg<sup>-1</sup> K<sup>-1</sup>,  $\kappa_{s1}=2$  W m<sup>-1</sup> K<sup>-1</sup>, and  $\phi_1=5/6$ . Material II (porous metal):  $\rho_{s2}=2700$  kg/m<sup>3</sup>,  $C_{s1}=800$  J kg<sup>-1</sup> K<sup>-1</sup>,  $\kappa_{s1}=230$  W m<sup>-1</sup> K<sup>-1</sup>, and  $\phi_2=5/6$ . Water:  $\rho_f=1000$  kg/m<sup>3</sup>,  $C_{f}=4200$  J kg<sup>-1</sup> K<sup>-1</sup>, and  $\kappa_f=0.6$  W m<sup>-1</sup> K<sup>-1</sup>. Other parameters are as follows:  $\Omega=0.03$  rad/s,  $r_1=3$  cm, and  $r_2=3.2$  cm.

temperature profile, the heaters and coolers should be taken away. Therefore, the thermal convection-conduction process is still passive, and we do not need to consider source terms in Eq. (1).

Without loss of generality, we set N = 4 and discuss  $N_1 = 2$  (allowed) and  $N_1 = 3$  (forbidden). Initial wave-like temperature profiles are presented in Figs. 4(b) and 4(e), and the results at t = 230 s are shown in Figs. 4(c) and 4(f). Line graphs and color graphs clearly indicate that the wave-like temperature profile with  $N_1 = 2$  can propagate stably, whereas that with  $N_1 = 3$  cannot (that is, its wavelength changes to  $N_1 = 1$ ). As a result, we may conclude that the thermal frequency modulator can be used to modulate or select the frequency of wave-like temperature profiles in thermal management.

We have achieved the prohibition and modulation of wave-like temperature profiles in an essentially one-dimensional case. Certainly, these results may be extended to two or three dimensions. Moreover, this work may broaden the methods of thermal management beyond transformation thermotics<sup>28–31</sup> and phononic engineering,<sup>4,32</sup> which may have potential applications in realizing thermal cloaking and camouflaging<sup>33–38</sup> according to the prohibition and modulation of wave-like temperature profiles, say, associated with the thermal frequency modulator.

In summary, we have reported the prohibition and modulation of wave-like temperature profiles with thermal convection-diffusion crystals. This phenomenon mainly originates from the convective effect in a periodic porous medium. These results may provide guidance to explore the frequency prohibition and modulation with thermal convection-diffusion dynamics and give insights into the development of other nonequilibrium systems, such as mass transport.<sup>39</sup>

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### DATA AVAILABILITY

The data that support the findings of this study are available within this article.

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