Anomalous energy diffusion and heat conduction in one-dimensional system*

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We propose a new concept, the centre of energy, to study energy diffusion and heat conduction in a one-dimensional hard-point model. For the diatom model, we find an anomalous energy diffusion as $\langle x^2\rangle \sim t^\beta$ with $\beta = 1.33$, which is independent of initial condition and mass rate. The present model can be viewed as the model composed by independent quasi-particles, the centre of energy. In this way, heat current can be calculated. Based on the theory of dynamic billiard, the divergent exponent of heat conductivity is estimated to be $\alpha = 0.33$, which is confirmed by a simple numerical calculation.

Keywords: energy diffusion, heat conduction, one-dimensional hard-point model
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1. Introduction

The link between the macroscopic thermodynamics and microscopic dynamics is an open problem in statistical physics. One important example of this subject is the heat conduction in the one-dimensional(1D) classic system. Much attention was devoted to identifying the sufficient condition of Fourier law.[1] One of the first analytic works showed that the heat conductivity κ in 1D harmonic lattice is divergent with system size L as $\kappa \sim L$, which violates Fourier law.[2] Recently, computer simulations have shown that some 1D models have anomalous heat conduction as $\kappa \sim L^\alpha$. However, the values of divergent exponent α obtained are different. For Fermi–Pasta–Ulam (FPU) model, α ranges from about 0.37 to 0.45.[1] For 1D diatom hard-point model, $\alpha = 0.33$ [3,4] and more smaller values, like $\alpha = 0.2$ to 0.25[5−7] are all reported. Simultaneously, several analytic attempts have been made to estimate the scaling law of κ. Self-consistent mode coupling theory[1] and Boltzmann equation[8] indicated that $\alpha = 2/5$ in 1D lattice system, while dynamical renormalisation group method[9] showed $\alpha = 1/3$ in 1D fluid-like system. These two analytic results are consistent with some simulation results of the FPU-β model and 1D diatom hard-point model, respectively. Some analytic studying and numerical simulations suggested that there may be two universality classes determined by the leading nonlinearity[10−12] and the transverse motion in 1D lattice model.[13,14] Recently, two different simulation results of the value of divergent exponent FPU-β model[15,16] were reported. The further study is needed to clarify this unsettled issue. To keep the valid of Fourier law in one-dimensional system, the effort of external on-site potential,[17] self-consistent reservoirs[18] and damping[19] were studied. It is believed that the destroyed momentum conservation should lead to normal heat conduction in one-dimensional system.[9]

On the other hand, some attempts were made to explore the relationship between the heat conduction and energy diffusion. To this end, one must first know their respective characters. Comparing with the study of heat conduction, the investigating of energy diffusion in 1D systems is lacking. Many degrees of freedom intrinsically in this kind of model prevent studying diffusion by tracking the dynamics of one particle. Nevertheless, there is another kind of 1D model called billiard channel model[20−23] which can also be used to study the heat conduction. This model is composed by the particles moving along a period array convex scatters. The interaction is absent between particles so that the model can be regarded as the ensemble of the single particle. If the thermal reservoirs are set at the borders of channel, the billiard

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system can model some characters of heat conduction in 1D many-body system. Furthermore, it also provides an opportunity to investigate the energy diffusion by studying the dynamics of billiard, which shows a diffusion character described by the mean square displacement as $\langle x^2(t)\rangle \sim Dt^{\beta}$. It is shown based on Levy walk theory that in billiard model there is a simple relation between β and the divergent exponent of heat conductivity α as $\alpha = \beta - 1$.[24] However, it is difficult to apply this result to the lattice model and the hard-point model directly because of the interaction between particles. Recently, by connecting the evolution of infinitesimal localised perturbation with energy diffusion, the energy diffusion in 1D hard-point model is studied.[25,26] A proof was made[25] that 1D diatomic hard-point model has diffusion character as well as Levy walk. As a result, $\alpha = 0.333$ was obtained. For 1D lattice models, the spatiotemporal correlation function of energy density fluctuation, treated as probability distribution function(PDF), was suggested to be used to calculate the scaling properties of energy diffusion and the numerical results showed that the relation $\alpha = \beta - 1$ is satisfied.[27]

In this paper, we propose a new prescription of energy quasi-particle, the centre of energy (CE), to study the energy diffusion, heat conduction and their relation directly in 1D hard-point model. We find an anomalous energy diffusion characterised by $t^{1.33}$ in the diatom model. The heat conduction in the present model can be understood based on the dynamics of single CE. As a result, the divergent exponent of heat conductivity in the diatom model is found to be 0.33.

2. Method and results

Before our starting, let us review the concept of the centre of mass(centroid). For a system composed of N particles, the centre of mass is a useful concept. It is defined as a point at which, for many purposes, the system's mass behaves as if it were concentrated. The displacement of the centre of mass is defined as $\boldsymbol{r}_c = (\sum_{i=1}^{N} m_i \boldsymbol{r}_i)/(\sum_{i=1}^{N} m_i)$, where m_i and $\boldsymbol{r}_i$ are the mass and displacement of the ith particle of system. In this way, the system can be treated as one particle with mass $M = \sum_{i=1}^{N} m_i$ and displacement $\boldsymbol{r}_c$. If we consider the energy diffusion in this system, we can not track back it to the motion of single particle. That is, these two kinds of motion are separated. However, as what we consider is energy diffusion and transport, it is desirable to find a new method, without considering the energy distribution of each particle. To this end, we introduce a new concept, the CE, whose displacement is defined as

$$\boldsymbol{r}_{\rm CE} = \frac{\sum_{i=1}^{N} \frac{1}{2} m_i {\boldsymbol{v}_i}^2 \boldsymbol{r}_i}{\sum_{i=1}^{N} \frac{1}{2} m_i {\boldsymbol{v}_i}^2}, \tag{1}$$

where $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$ are the displacement and velocity of the ith particle. The physical meaning of CE is that the total energy of all particles is concentrated on a point. The coordinate of CE is a weighted mean of coordinates of each particle and the weighting is the energy of particle. When the system is in equilibrium state, the displacement of the CE should be fixed. On the contrary, when system is in non-equilibrium state, the displacement of CE will change as time goes by until the equilibrium state is reached. In the following, we will employ this new concept to the studying of energy diffusion and transport in 1D hard-point model.

1D hard-point model consists of a chain of N particles with mass m_i lying on a segment of length L. The motion of particles is restricted to one dimension so that they can not be exchanged with each other. The displacements of particles satisfy the condition $0 < x_1 < x_2 \ldots x_i < x_{i+1} \ldots x_N < L$. The interaction between two adjacent particles is elastic collision with total energy and momentum conserved. Denoting the velocity of ith particle before(after) a collision by $v_i(v_{i'})$, the velocity evolution is given by linear equation

$$\begin{aligned} v_i' &= \frac{m_i - m_{i'}}{m_i + m_{i'}} v_i + \frac{2m_{i'}}{m_i + m_{i'}} v_{i'}, \\ v_{i'}' &= \frac{2m_i}{m_i + m_{i'}} v_i - \frac{m_i - m_{i'}}{m_i + m_{i'}} v_{i'}, \end{aligned} \tag{2}$$

where i' denotes $i+1$ or $i-1$. The energy of one particle is $e_i = m_i v_i^2/2$ and the total energy of model is $E = \sum_{i=1}^{N} e_i$. The local temperature is defined as $T_i = \langle m_i v_i^2 \rangle / k_{\rm B}$, where $k_{\rm B}$ is Boltzmann constant.

For Eq. (2), considering a simple case that $v_{i'} = 0$, we obtain

$$\begin{aligned} v_i' &= \frac{m_i - m_{i'}}{m_i + m_{i'}} v_i, \\ v_{i'}' &= \frac{2m_i}{m_i + m_{i'}} v_i. \end{aligned} \tag{3}$$

Otherwise, in the case that $v_i = 0$, we obtain

$$\begin{aligned} v_i' &= \frac{2m_{i'}}{m_i + m_{i'}} v_{i'}, \\ v_{i'}' &= -\frac{m_i - m_{i'}}{m_i + m_{i'}} v_{i'}. \end{aligned} \tag{4}$$

We notice that the superposition of Eq. (3) and Eq. (4) leads to the Eq. (2). That is, the velocity evolution in Eq. (2) can be decomposed into two collision evolution in Eq. (3) and Eq. (4). It can be seen easily that superposition of velocity is linear, which indicates that two velocity evolutions in Eq. (3) and Eq. (4) are independent.

For whole system, assume at one time t, the velocity distribution of all particles can be described by the function $f(v_1, v_2, \ldots v_i, \ldots, v_N)$ and the displacement distribution of particles can be described by $g(x_1, x_2, \ldots, x_N)$. We assume that an arbitrary velocity distribution at time t with same $g(x_1, x_2, \ldots, x_N)$ is $\phi_j(v_1^j, v_2^j, \ldots v_i^j, \ldots, v_N^j)$ which is the evolution resulted from a certain initial condition. Due to the linear superposition of velocity in Eq. (2), we can expand $f(v_1, v_2, \ldots v_i, \ldots, v_N)$ as

$$\begin{aligned} & f(v_1, v_2, \ldots v_i, \ldots, v_N) \\ &= \sum_{j=1}^{\infty} a_j \phi_j(v_1^j, v_2^j, \ldots v_i^j, \ldots, v_N^j), \end{aligned} \tag{5}$$

where the functions $\phi_j(v_1^j, v_2^j, \ldots v_i^j, \ldots, v_N^j)$ should compose an infinite orthogonal complete set because of the infinite initial condition. Considering the properties of this model, the arbitrary initial condition of system has fixed momentum $P_j = \sum_{i=1}^{N} p_i$ and energy $E_j = \sum_{i=1}^{N} e_i$, which will be kept during the evolution from this initial condition because of the conservation of momentum and energy. In term of the definition (1), such evolution of a state of the model can be described by the motion of CE with momentum P_j and energy E_j. That is, we can treat CE as a quasi-particle. Due to the independence of CE, we can investigate the thermal properties of this model by studying the motion of CE.

Considering the heat conduction in 1D hard-point model, two heat baths are usually connected to the two ends. The leftmost and rightmost particles can collide with them and energy is exchanged between the model and the heat bathes through collisions. That is, any state of model in thermal process can be approached by these collisions. Assuming the initial condition is that the model is in its ground state with zero momentum and fixed displacement distribution, we connect a heat bath with the left end of the model and switch it off once after it collides with the leftmost particle. This particle will obtain a velocity toward the opposite end of model and move with a constant speed until it collides with the second particle. Subsequently, more collisions will occur among more particles and a state of model is approached at time t. If the initial displacement distribution of all particles is different, the reached state at time t is different. We can choose these states of the model at time t as the function set to expand an arbitrary state at same time. Then the energy obtained by the leftmost(rightmost) particle after one collision with heat bath can be defined as the energy of quasi-particle, whose dynamics can be described by the motion of CE, which give the motion of each set function. Therefore, the process of energy exchange between the model and the heat bath is equivalent to the exchange of CE.

We first consider a simple case of 1D hard-point model that the initial displacements of particles are set $x_i = i \times a$, where a is the average distance of particles. Without losing generality, we set $a = 1$ in this study. All particles are static, except the first one with a nonzero velocity v_0 obtained from a collision with the heat bath. Fixed boundary condition is applied.

When the present model is integrable that each particle has same mass $m_i = m_0$, the two particles will exchange their velocities after a collision. If the velocity of one particle is zero before collision, it will obtain the velocity of the other one by colliding, while the other one loses its momentum. That is, the energy is transferred completely from one to one and will always concentrate at one particle. In this case, CE is simple. If the velocity of the leftmost particle obtained from heat bath is v_0, CE will move with the constant velocity v_0 and its displacement evolutes with dynamics equation $x_c = v_0 t$. That is , the square displacement is $\langle x_c^2 \rangle \sim t^\beta$ and $\beta = 2$, which indicates a ballistic diffusion.

Next, we consider the diatom model which is no longer integrable. The masses of particles are $m_{2i} = m_0$, $i = 1, 2 \ldots [N/2]$ and $m_{2i+1} = r m_0$, $i = 0, 1, \ldots [(N-1)/2]$, r is the mass rate. We first take mass rate to be gold number, $r = \sqrt{5} - 1/2$. The diffusion behaviour of CE in this case is showed in Fig. 1. We find that the square displacement scales like $\langle x^2 \rangle \sim t^\beta$ and $\beta = 1.33$, which is smaller than that of ballistic case. As the adjacent particles have different mass, only part of energy of one particle can be transported to the other one during a collision. This plays a role like the barrier in the billiard channel, which leads to the anomalous diffusion. The motion of CE in the model with other mass rates is also studied. Some results are presented in Table 1. We find

that the diffusion exponent β are all approximate 1.33.

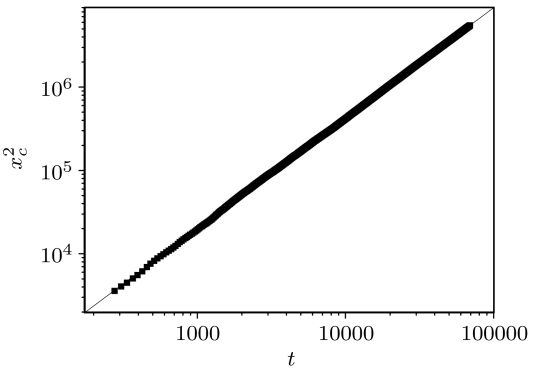


Fig. 1. Square displacement of CE as a function of time. The fit is $x_c^2 \sim t^\beta$, $\beta = 1.33$. The system size is $N = 4000$ and fixed boundary condition is applied. The initial velocity is $v_0 = 1.0$. Mass rate is $r = (\sqrt{5}-1)/2$.

Table 1. Energy diffusion exponent β of the hard-point model with different mass rates and different initial conditions. The system size is $N = 4000$ and fixed boundary condition is applied. The initial velocity is $v_0 = 1.0$. The total evolution time is the time sum of 2×10^7 collisions.

mass rate	1/3	2/5	1/2	$(\sqrt{5}-1)/2$	$\sqrt{2}/2$
β(uniform)	1.334	1.330	1.336	1.326	1.326
β (general)	1.335	1.330	1.334	1.331	1.330

We also investigate the motion of CE with the general initial condition. The initial displacements of particles are set stochastically as $x_i = i + \delta_i$, where δ_i is the uniform random number in the region $(-1, 1)$. However, the chose of x_i guarantees the condition $0 < x_1 < x_2 \ldots x_i < x_{i+1} \ldots x_N < L$. We investigate the dynamics of CE in some different mass rate cases. The results are also showed in Table 1. It is noted that the diffusion exponents are all close to 1.33. Tracing the motion of CE with different initial condition, we find the order of collision among particles is different, which means that the detail motion of CE with different initial condition are different, but diffusion law is independent of initial condition, i.e. the collision order.

It is well known that the velocity of particles should satisfy Maxwell's distribution when the local thermal equilibrium state is reached in heat conduction. The energy diffusion of CE should be averaged on velocity distribution. It can be seen easily that when the initial velocity varies, the collision order will not change while the time for finish same collision will change. Assuming the initial velocity of first particle and the distance between the first and second particles are v_0 and l, then the time for the first collision is $t_1 = l/v_0$. When the initial velocity becomes αv_0, then the time becomes t_1/α. The subsequently collision will change in the same way. That is, the CE with a large initial velocity will move faster than the one with small velocity, but the diffusion laws of CEs are the same, which is not dependent on initial velocity when the initial displacement of all particles are the same. This supports the idea[24] that for 1D hard-point model, any heat bath is equivalent and can be replaced by a simple 'delta' heat bath with the probability density function, $P_T(\varepsilon) = \delta(\varepsilon - \sqrt{T/2})$.

We have investigated the properties of single CE generated by a kick on the end of model in zero temperature limit. As discussed early, the heat conduction in this model can be decomposed into the motion of independent CEs. This provides a new method to study the heat conduction in 1D hard-point model. Considering the model connected with heat bath, during the time t, the energy transferred from the heat bath to the model can be written as

$$Q(t) = \sum_{i=1}^{M(t)} \varepsilon_i, \tag{6}$$

where $M(t)$ is the total number of CE propagating along the model during time t. ε_i is the energy of ith CE. Hence, the heat current can be written

$$J = \lim_{t\to\infty} \frac{Q(t)}{t}. \tag{7}$$

To estimate the heat current, we first consider the contribution of one CE whose energy, here, is denoted by ε. The heat current of a CE is $j = \varepsilon/t$. The average energy carried by a CE is $\int_0^\infty \varepsilon P(\varepsilon)\mathrm{d}\varepsilon$, where $P(\varepsilon)$ is the energy distribution of heat bath. In this way, the problem of heat transport can be treated as the diffusion of CE. Taking into account the thermodynamic velocity, the time τ for CE to reach an opposite end should be averaged. As discussed early, the diffusion law is not dependent on the velocity of CE and the 'hot' one just passes the model faster than the 'cold' one, and the arrival time of the CE should be rescaled by the energy factor as $\tau \longrightarrow \tau \int_0^\infty (1/\sqrt{2\varepsilon})\sqrt{m} P_{T_\pm}(\varepsilon)\mathrm{d}\varepsilon$. As a result, the average heat current contributed by one CE can be written as

$$j = \tau^{-1} \left(\frac{\int \varepsilon P_{T_+}(\varepsilon)\mathrm{d}\varepsilon - \int \varepsilon P_{T_-}(\varepsilon)\mathrm{d}\varepsilon}{\int \frac{\sqrt{m}}{\sqrt{2\varepsilon}} P_{T_+}(\varepsilon)\mathrm{d}\varepsilon + \int \frac{\sqrt{m}}{\sqrt{2\varepsilon}} P_{T_-}(\varepsilon)\mathrm{d}\varepsilon} \right). \tag{8}$$

The heat current carried by N CEs is $J = Nj$. When the temperature of heat baths is fixed, the temperature profile is also fixed so that the density of CEs in

the model should be constant and N should be proportional to the length of model L as $N \sim L$.

The dependence of heat current on the length of model can be estimated by investigating the relation between the average arrive time for CE and the length of model. In Ref. [24], treating the dynamical billiard channel as random walk model due to the diffusion-like dynamics of billiard, authors estimated the arrival time versus the length of channel and found a simple relation between the divergent exponent of heat conductivity and the anomalous diffusivity exponent as $\alpha = \beta - 1$. In our study of hard-point model, energy diffusion can be described by the motion of CE which shows diffusion character as well as the billiard in channel. So we can apply the relation $\alpha = \beta - 1$ to our results and find easily that the divergent exponent of heat conductivity turns out to be 0.33, which is in perfect agreement with the numerical results[3,4] and the result of dynamical renormalisation group method.[9]

Except for the analytic method, we can estimate the heat current by calculating the arrival time τ directly. In ballistic case, the energy is always staying at one point, the arrive time can be calculated from the diffusion law of CE so that $\tau = t = L/v_0$. Taking it into formula (5), we obtain $J \sim L^0$. Upon substituting J into Fourier law, we find $\kappa \sim L$, which consists with the analytic result and simulation result. In the diatom case, we can still calculate time based on diffusion law: $t \sim L^{2/\beta}$, but we can not treat it as the arrival time of CE τ because of the following reasons. First, our derivation of formula (5) is based on the closed boundary condition, which means that the energy of CE is conserved. However, in thermal transport, the model is connected with the heat baths and the boundary is open. CE will lose energy during propagating by continuous colliding with the boundary so that the energy of CE in formula (5) is not constant. Actually, this is the reason for the formation of temperature profile. When the masses of particles are uniform, CE will not lose energy before it reach the opposite end so that the temperature profile can not form. Second, as CE represents the energy distribution, when the font of distribution packet touches the opposite end and exchanges energy with it, the motion of CE should be altered strongly by the boundary and will not behave as $t^{1.33}$.

Due to these reasons, the calculation of arrive time is difficult. Here, we just make a simple estimation. We make an approximation that the energy of CE is constant during the propagation. In Fig. 2, we plot the motion of the CE and note that when it reaches the opposite end of model, it will be rebounded. We assume the arrival time as the time for CE when it is rebounded at first time. The system size of model as a function of arrival time is plotted in Fig. 3. The fitting indicates a power law as $L \sim t^{\eta}, \eta = 0.608$, which is very close to 3/5 but smaller than $\beta/2 = 2/3$ calculated from diffusion law directly.

We also calculate η for different mass rates with random initial condition (showed in Table 2). The results are all close to 3/5. Then the arrival time $\tau \sim L^{1/\eta}$. Upon substituting it into the formula of heat current and denoting $1/\eta$ by γ, we can find

$$J(L) \sim L^{1-\gamma}. \tag{9}$$

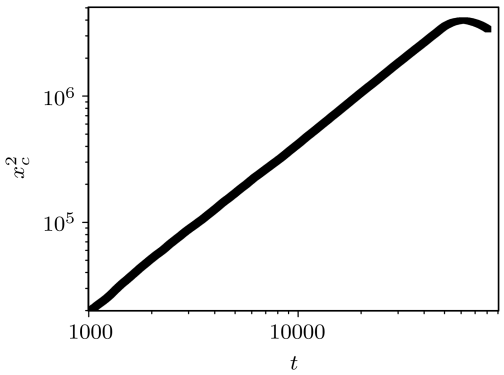


Fig. 2. Square displacement of CE as a function of time when time t is long enough. The system size is $N = 2000$ and the fixed boundary condition is applied. The initial velocity is $v_0 = 1.0$. Mass rate is $r = (\sqrt{5} - 1)/2$.

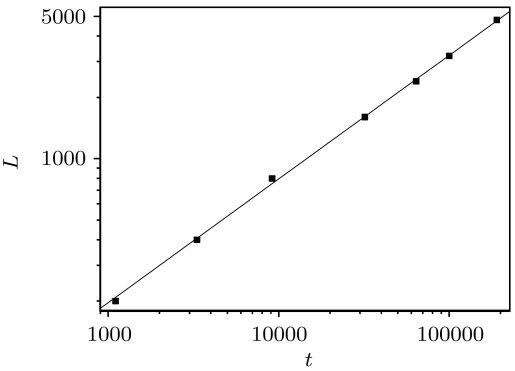


Fig. 3. Length of system versus the first arrival time. The fit scale is $L \sim t^{\eta}$,$\eta = 0.608$. The mass rate is $r = (\sqrt{5} - 1)/2$, the initial velocity of CE is $v_0 = 1$.

Table 2. The divergent exponent η as the function of system size of 1D hard-point model for the different mass rates and general initial condition.

mass rate	1/3	2/5	1/2	$(\sqrt{5}-1)/2$	$\sqrt{2}/2$
η	0.604	0.609	0.607	0.602	0.603

Taking account of the Fourier law $\kappa = -J \times L/\triangle T$, we can estimate the heat conductivity. The result is

$$\kappa \sim L^{2-\gamma}. \tag{10}$$

The divergence is in the thermodynamics limit $L \to \infty$. In our simple estimating, $\gamma = 1/\eta \approx 1.67$, so $\kappa \sim L^{0.33}$, which coincides with our early analytic result and is also in agreement with the previous numerical simulation result[3,4] and the renormalisation group result.[9]

3. Summary

In summary, we introduced a new concept, CE, to investigate the energy diffusion and heat conduction in 1D hard-point model. By considering a kick excitation from the ground state of this classic model, we found an anomalous energy diffusion behaving as $t^{1.33}$ in the diatom case. The simulation also showed the independence of diffusion law on the initial condition and mass rate. As a result, the heat conduction hard model can be studied by investigating the dynamics of CE. We found that the heat conduction is also anomalous and heat conductivity is divergent with system size as $\kappa \sim L^{\alpha}$. Applying the relation between the diffusion exponent and the divergent exponent of heat conductivity in the dynamic billiard model to 1D hard-point model, we found that the divergent exponent α turns out to be 0.33, which is confirmed by a simple numerical estimation.

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