Microscopic Energy Flux in Particle Systems and Nonlinear Lattices

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We study the distribution of the microscopic energy flux \( j \) which is carried by a single particle. It is observed in Lennard-Jones particle system that the distribution of the norm of the energy flux \( P_n(j) \) has a broad peak in small \( j \) regime and a stretched-exponential decay for large \( j \). The broad peak originates in the potential advection and energy transfer between particles. The stretched exponential tail is from the momentum energy advection. In nonlinear-lattice systems, all the flux components \( j_K, j_U, \) and \( j_F \) show stretched exponential decay.

§1. Introduction

A good lesson from the great success of molecular dynamics simulations in the last half a century is the importance of observing fine quantities directly, which are virtually impossible in experimental and theoretical physics. One of the most prominent examples is the discovery of the long-time-tails of the velocity-autocorrelation function in hard-core particle systems.1)–5) The relevance of these findings on transport phenomena is again highlighted in the last decade in the studies of anomalous conductivity in momentum conserving nonlinear lattices.6)–16)

Here we study the distribution of microscopic energy flux, which is carried by a single particle. The heat flux is expected to be a good measure to characterize the nonequilibrium steady states with temperature gradient. However, there tends to remain no good information in the distribution of ordinary local energy flux \( \mathbf{J} = \frac{1}{V} \sum_i j_i \), where \( j_i \) denotes the energy flux carried by each particle in the volume element \( V \), hence the summation is taken for the particles in the volume. The characteristic Gaussian distribution which is widely observed in a system in thermal equilibrium, as shown in Fig. 1, and the one with shifted peak position observed in nonequilibrium steady state with nonzero average flux, are simply the consequence of the central limit theorem. Therefore, for instance, it is fruitless to argue the fluctuation theorem on such quantities. However, we can find characteristic distribution forms in much finer scale: the distributions of the flux carried by a single particle and the flux on a single bond (see Fig. 1, right). This is why we here focus on the single-particle and single-bond fluxes. For systems with potentials, the local energy flux \( \mathbf{J} \) may not be determined solely from the distribution of single particle flux \( \mathbf{j} \), since the correlation among them may be relevant. Yet the single-particle distribution is still essential for local flux and is a good observable for simulational physics.
§2. The equilibrium energy flux distribution in a particle system

Let us consider systems with two-body potential as

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m^2} + \sum_{i<j} U_{ij}(q_i, q_j). \quad (2.1)$$

The energy flux transported by a particle \(i\) in such systems can be expressed as

$$\mathbf{j} = \frac{p_i^2 \mathbf{p}_i}{2m^2} + \sum_j \left\{ \frac{U_{ij} \mathbf{p}_i}{2m} - (q_i - q_j) \left( \frac{\partial U_{ij}}{\partial q_i} \cdot \frac{\mathbf{p}_i}{m} \right) \right\}. \quad (2.2)$$

The first term represents the advection of the kinetic energy. The second and third terms come from the interaction and they denote the advection of the local potential energy and the energy transfer via the potential force, respectively. In the following, we will denote those three flux terms as

$$\mathbf{j} = \mathbf{j}_K + \mathbf{j}_U + \mathbf{j}_F$$

with

$$\mathbf{j}_K = \frac{p_i^2}{2m^2} \mathbf{p}_i, \quad \mathbf{j}_U = \sum_j \frac{U_{ij} \mathbf{p}_i}{2m}, \quad \text{and} \quad \mathbf{j}_F = - \sum_j (q_i - q_j) \left( \frac{\partial U_{ij}}{\partial q_i} \cdot \frac{\mathbf{p}_i}{m} \right). \quad (2.3)$$

2.1. The kinetic energy advection term

From the equilibrium distribution of momentum

$$P_d(p) = \left( \frac{\beta}{2m \pi} \right)^{\frac{d}{2}} \exp \left\{ - \frac{\beta p^2}{2m} \right\}, \quad (2.4)$$

where \(d\) and \(\beta = (k_B T)^{-1}\) represent the dimensionality of the momentum space and the inverse temperature, the distribution of the kinetic advection in thermal equilibrium is straightforwardly obtained as

$$P_d(j_K) \, dj_K = \frac{P_d(p)}{j^d_{j=p}} \frac{dp}{j^{d-1}j} = \frac{1}{3} \left( \frac{\beta'}{\pi} \right)^\frac{d}{2} \exp \left\{ -\beta' j_K^2 \right\} \left( \frac{\beta'}{j_K^2} \right)^{\frac{d}{2}} \, dj_K \quad \left( \beta' = \left( \frac{m}{2} \right)^{\frac{1}{2}} \beta \right), \quad (2.5)$$
where $j_K$ denotes the flux norm $|j_K|$ and the Jacobian is calculated as $J_{j→p}^d = 3 \left( \frac{e^2}{2m^*} \right)^d = 3 \left( \frac{e^2}{2m^*} \right)^{\frac{d}{2}}$. What is important in this naïve calculation is that the distribution of the kinetic advection term has a stretched exponential dependence and an algebraic singularity at $j_K = 0$. It is also useful for fitting the simulation data since some of the distribution forms we list in the following are simple.

### 2.1.1. Distribution of the norm of $j_K$

From Eq. (2.5) the distribution for the flux norm, which we denote as $P^n_d$ in the following, is calculated as

$$P^n_d(j_K) = \left( \frac{2\beta'^{\frac{d}{2}}}{3\Gamma(\frac{d}{2})} \right) j_K^{\frac{d-3}{d}} \exp \left\{ -\beta' j_K^{\frac{2}{3}} \right\}, \quad \text{(2.6)}$$

or, specifically to each dimension,

$$P^n_1(j_K) = \left( \frac{2\beta'}{3\sqrt{\frac{3}{\pi}}} \right) \frac{\exp\{-\beta' j_K^{\frac{2}{3}}\}}{j_K^{\frac{1}{3}}}, \quad \text{(2.7)}$$

$$P^n_2(j_K) = \left( \frac{2\beta'}{3} \right) \frac{\exp\{-\beta' j_K^{\frac{2}{3}}\}}{j_K^{\frac{1}{3}}}, \quad \text{(2.8)}$$

$$P^n_3(j_K) = \left( \frac{4\beta'}{3\sqrt{\pi}} \right) \frac{\exp\{-\beta' j_K^{\frac{2}{3}}\}}{j_K^{\frac{1}{3}}}, \quad \text{(2.9)}$$

$$P^n_4(j_K) = \left( \frac{2\beta'^{\frac{2}{3}}}{3} \right) j_K^{\frac{1}{3}} \exp\{-\beta' j_K^{\frac{2}{3}}\}; \quad \text{(2.10)}$$

$$\vdots$$

etc. The norm distributions also have singularity at $j_K = 0$ in one- and two-dimensional systems. The simple stretched exponential form for three-dimensional systems is found to be useful to investigate the distribution in nonequilibrium.\textsuperscript{17}

### 2.1.2. Distribution of a cartesian component of $j_K$

The distribution of a certain cartesian component, denoted as $P^n_d(j_{Kj})$, would be more interesting especially to approach to the understanding of nonequilibrium state. However, for $d ≥ 2$, the distribution is calculated as

$$P^n_d(j_{Kj}) = \int_0^\infty 2\beta'^{\frac{d}{2}} r^{d-2} \exp \left[ -\beta' \left\{ (j_{Kj})^2 + r^2 \right\}^{\frac{1}{2}} \right] dr \quad \text{(2.11)}$$

$$= \frac{\beta'^{\frac{d}{2}}}{\sqrt{\pi} \Gamma(\frac{d-1}{2})} \left( j_{Kj}^{\frac{2}{3}} \right)^{\frac{d-3}{2}} \int_0^\infty \exp\{-\beta' t\} dt, \quad \text{(2.12)}$$

or, specifically,

$$P^n_1(j_{Kj}) = \left( \frac{1}{3\sqrt{\frac{3}{\pi}}} \right) \frac{\exp\{-\beta' (j_{Kj})^{\frac{2}{3}}\}}{(j_{Kj})^{\frac{1}{3}}}, \quad \text{(2.13)}$$
Microscopic Energy Flux

\[ P_2^x(j_K^x) = \frac{\beta'}{\pi} \int_0^\infty \frac{\exp\{-\beta' t\}}{\sqrt{t^3 - (j_K^x)^2}} \, dt, \quad (2.14) \]

\[ P_3^x(j_K^x) = \frac{\beta' \pi}{2} \int_0^\infty \frac{\exp\{-\beta' t\}}{t^2} \, dt = \frac{\beta' \pi}{2} \frac{\text{Ei}(-\beta' (j_K^x)^2)}{2}, \quad (2.15) \]

\[ P_4^x(j_K^x) = \frac{2\beta^2}{\pi} \int_0^\infty \frac{\sqrt{t^3 - (j_K^x)^2}}{t^2} \exp\{-\beta' t\} \, dt. \quad (2.16) \]

2.2. Potential-derived terms

Since there is no correlation between the distributions of momenta and coordinates in the equilibrium ensemble of classical system, the expectation value of the flux for a given momentum \( p \) can be written as

\[ \langle j(p) \rangle_q = \frac{p^2 \mathcal{P}}{2m^2} + (\Psi_U + \Psi_F) \cdot p \equiv j_K + \langle j_U \rangle_q + \langle j_F \rangle_q, \quad (2.17) \]

where \( \langle \rangle_q \) denotes the ensemble average over coordinate space, and \( \Psi_U \) and \( \Psi_F \) are calculated as

\[ \Psi_U(\beta) = \frac{\langle \sum_j U_{ij} \rangle_q}{2m}, \quad (2.18) \]

\[ \Psi_F(\beta) = \left\langle -\frac{1}{m} \sum_j \left\{ (q_i - q_j) \frac{\partial U_{ij}}{\partial q_i} \right\} \right\rangle_q, \quad (2.19) \]

respectively.

The equilibrium distributions of the norm of the flux components, \( \tilde{j}_\alpha \equiv |\langle j_\alpha \rangle_q| \) (\( \alpha \) is for \( U \) or \( F \)) are calculated as

\[ P(\tilde{j}_\alpha) = \frac{2}{\Gamma\left(\frac{d}{2}\right)} \left( \frac{\beta}{2(m|\Psi_\alpha|)^2} \right)^{\frac{d}{2}} (\tilde{j}_\alpha)^{d-1} \exp\left\{ -\frac{\beta}{2m^2|\Psi_\alpha|^2} (\tilde{j}_\alpha)^2 \right\}, \quad (2.20) \]

where \( |\Psi_F| \) denotes \( \left| \frac{\text{tr}(\Psi_F)}{2} \right| \) (the factor \( \frac{1}{2} \) comes from taking an average of product of vectors with independent directions). We expect that this \( \tilde{j}_\alpha \), which stems from the potential and has \( p \)-first order form, becomes relevant for small \( p \), and hence for small \( j \). Note that the width of the distribution of the flux itself is expected to be broader than the one of \( \tilde{j}_\alpha \) since \( j_\alpha \) is a product of \( p \) and potential-related term.

2.3. Distribution of total energy flux

Equations (2.9), (2.17), and (2.20) imply that the distribution of the total local energy flux norm \( P(j) \) of three-dimensional particle systems typically shows crossover from Maxwell distribution region, in which potential term is dominant, to non-Maxwellian region, in which momentum energy advection is dominant. That is actually what we see in Lennard-Jones particle system (Fig. 2).\(^{18}\) The peak position of the distribution is confirmed to be consistent with the one predicted from the analytically estimated \( |\Psi_\alpha| \). We can also confirm that our argument is valid for liquid and solid phases (Fig. 3), although it is difficult to give \( |\Psi_\alpha| \) independently from the simulation.
Fig. 2. The distribution of the norm of the single particle energy flux (given in Eq. (2.2)) obtained from a Lennard-Jones particles system in the super critical fluid phase. The dotted line represents the distribution for hard-core particles (Eq. (2.9)).

Fig. 3. The equilibrium distribution function of the single particle energy flux in Lennard-Jones liquid (left) and solid (right). Theoretical lines are obtained from fitting using the Maxwellian form.

§3. The equilibrium energy flux distribution in nonlinear lattices

In the previous section, we found a good explanation for the equilibrium distribution of the flux by treating the averaged flux instead of the flux itself. However, in the systems which have very small $|\Psi_\alpha|$, our approximation may not be valid. The nonlinear lattice and lattice-like systems are such examples. Here we first use the one-dimensional FPU-\(\beta\) lattice.

It turns out that the distribution obtained from the one-dimensional FPU-\(\beta\) lattice does not show the Gaussian peak at \(j = 0\) which is expected from Eq. (2.20). Furthermore, it is found that both the potential-originated flux components \(j_U\) and
Microscopic Energy Flux

Fig. 4. The distribution of the single bond energy flux in the one-dimensional FPU-β lattice (left) and three-dimensional systems with connections of \((N_x \times N_y \times N_z)\) (right). The periodic boundary condition is imposed for \(x\)- and \(y\)-directions in the latter cases. Dotted lines in the left figure represents the fitting by Eq. (2.7).

\(j_F\) show kinetic-term like stretched exponential form (see Fig. 4, the left panel).

Since the one-dimensional FPU-beta lattice is known to exhibit anomalous thermal conduction, it is tempting to ask whether the peculiar equilibrium distribution is related to the existence of the non-diffusive transport. It is known that the three-dimensional system whose Hamiltonian is given as the following equations shows anomalous behavior when the connection is one-dimensional and reproduces normal thermal conduction when the connection is three-dimensional:

\begin{align}
\mathcal{H} &= \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i,j,\text{n.n}} V_{ij}, \\
V_{ij} &= \frac{k}{2} (dq_{ij})^2 + \frac{g}{4} (dq_{ij})^4 , \quad (dq_{ij} = |q_i - q_j| - l_0) \tag{3.2}
\end{align}

where \(N, l_0\), and \(g\) denote the number of particles, the natural length of the bonds, and the parameter of 4th order nonlinear term respectively and the summation over \(V_{ij}\) takes only for nearest neighbor pairs. In the right panel in Fig. 4, we can see that the peculiar kinetic-term like distributions is also observed in the systems which shows normal heat conduction. A slight systematic difference between one dimensionally coupled system and three dimensionally coupled systems might be related to the anomalous transport.

§4. Conclusions

We have focused on the distribution of the single-particle and single-bond energy flux \(j\). We first derived the distributions of the three flux terms for particle systems and predict the distribution profile of the total flux with a crossover from the potential-originated Maxwellian region to the stretched exponential tail, which comes from the kinetic energy advection term. Using a Lennard-Jones particle system, the cross-over profile is numerically confirmed in gas, liquid, and solid states. In nonlinear-lattice systems, however, all the flux components show kinetic-term like
distribution.

An interesting question based upon those results is how the flux distribution will be modulated when the system is not in equilibrium, i.e. how the energy flows microscopically. We can find that the kinetic advection term again plays a dominant role in the nonequilibrium steady state with temperature gradient.\textsuperscript{17}

**References**